arXiv:1007.1076v6 [math.AG] 23 Nov 2011

EXPLICIT ASSOCIATOR RELATIONS FOR MULTIPLE ZETA VALUES

ISMAEL SOUDÈRES

ABSTRACT. Associators were introduced by Drinfel'd in [Dri91] as a monodromy representation of a Knizhnik-Zamolodchikov equation. Associators can be briefly described as formal series in two non-commutative variables satisfying three equations. These three equations yield a large number of algebraic relations between the coefficients of the series, a situation which is particularly interesting in the case of the original Drinfel'd associator, whose coefficients are multiple zetas values. In the first part of this paper, we work out these algebraic relations among multiple zeta values by direct use of the defining relations of associators. While well-known for the first two relations, the algebraic relations we obtain for the third (pentagonal) relation, which are algorithmically explicit although we do not have a closed formula, do not seem to have been previously written down. The second part of the paper shows that if one has an explicit basis for the bar-construction of the moduli space $\mathcal{M}_{0,5}$ of genus zero Riemann surfaces with 5 marked points at one's disposal, then the task of writing down the algebraic relations corresponding to the pentagon relation becomes significantly easier and more economical compared to the direct calculation above. We discuss the explicit basis described by Brown, Gangl and Levin, which is dual to the basis of the enveloping algebra of the braids Lie algebra $U\mathfrak{B}_5$.

In order to write down the relation between multiple zeta values, we then remark that it is enough to write down the relations associated to elements that generate the bar construction as an algebra. This corresponds to looking at the bar construction modulo shuffle, which is dual to the Lie algebra of 5-strand braids. We write down, in the appendix, the associated algebraic relations between multiple zeta values in weights 2 and 3.

CONTENTS

Date: November 24, 2011.

I want to thank Leila Schneps, Pierre Cartier for their support, their kind attention to my work and all the discussions that lead to this article. Benjamin Collas was a great help in mastering the computer, relations in the annexe being computed using Mathematica. I also want to thanks particularly Francis Brown for all his important and useful comments.

1. Introduction

In the first part of this introduction we recall the necessary definitions concerning associators, and in the second part, we recall the definitions and main results concerning multiple zeta values. In the third part, we give the outline of the paper and state the main results.

1.1. Associators.

Let k be a field of characteristic 0. Let $U\mathfrak{F}_2 = k\langle\langle X_0, X_1\rangle\rangle$ be the ring of formal power series over k in two non-commutative variables. The coproduct Δ on $U\mathfrak{F}_2$ is defined by

$$\Delta(X_0) = X_0 \otimes 1 + 1 \otimes X_0 \qquad \Delta(X_1) = X_1 \otimes 1 + 1 \otimes X_1.$$

An element $\Phi = \Phi(X_0, X_1) \in U\mathfrak{F}_2$ is *group-like* if it satisfies $\Delta(\Phi) = \Phi\hat{\otimes}\Phi$ where $\hat{\otimes}$ denotes the complete tensor product.

Remark 1.1. We remark that the constant term of a group-like element is 1.

Definition 1.2. If S is a finite set, let S^* denote the set of words with letters in S, that is the dictionary over S. If $S = \{s_1, \dots, s_n\}$ we may write $\{s_1, \dots, s_n\}^*$.

Let $\mathcal{W}_{0,1}$ be the dictionary over $\{X_0, X_1\}$.

We remark that the monomials in $U\mathfrak{F}_2$ are words in $\mathcal{W}_{0,1}$; the empty word $\emptyset$ in $\mathcal{W}_{0,1}$ will be 1 by convention when considered in $U\mathfrak{F}_2$. The following definition allows us to define a filtration on $U\mathfrak{F}_2$.

Definition 1.3. The depth $dp(W)$ of a monomial $W \in U\mathfrak{F}_2$, that is an element of $\mathcal{W}_{0,1}$, is the number of X_1's, and its weight (or length) $wt(W) = |W|$ is the number of letters.

The algebra $U\mathfrak{F}_2$ is filtered by the weight, and its graded pieces of weight d are the subspaces generated by the monomials of length d; $U\mathfrak{F}_2$ is thus a graded algebra.

Let $U\mathfrak{B}_5$ be the enveloping algebra of $\mathfrak{B}_5$, the completion (with respect to the natural grading) of the pure sphere braid Lie algebra [Iha90]; that is, $U\mathfrak{B}_5$ is the quotient of $k\langle\langle X_{ij}\rangle\rangle$ with $1 \leqslant i \leqslant 5$ and $1 \leqslant j \leqslant 5$ by the relations

- $X_{ii} = 0$ for $1 \leqslant i \leqslant 5$,
- $X_{ij} = X_{ji}$ for $1 \leqslant i, j \leqslant 5$,
- $\sum_{j=1}^{5} X_{ij} = 0$ for $1 \leqslant i \leqslant 5$,
- $[X_{ij}, X_{kl}] = 0$ if $\{i, j\} \cap \{k, l\} = \emptyset$.

Definition 1.4 (Drinfel'd [Dri91])**.** A group-like element Φ in $U\mathfrak{F}_2$ having coefficients equal to zero in degree 1, together with an element $\mu \in k^*$, is an associator if it satisfies the following equations

$$\Phi(X_0, X_1)\Phi(X_1, X_0) = 1, \tag{I}$$

$$e^{\frac{\mu}{2}X_0}\Phi(X_\infty, X_0)e^{\frac{\mu}{2}X_\infty}\Phi(X_1, X_\infty)e^{\frac{\mu}{2}X_1}\Phi(X_0, X_1) = 1, \tag{II}$$

with $X_0 + X_1 + X_\infty = 0$, and

$$\Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{51}, X_{12})\Phi(X_{23}, X_{34})\Phi(X_{45}, X_{51}) = 1, \tag{III}$$

where (III) takes place in $U\mathfrak{B}_5$.

We will write an associator as

$$\Phi(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} Z_W W = 1 + \sum_{\substack{W \in \mathcal{W}_{0,1} \\ W \neq \emptyset}} Z_W W.$$

We have $Z_\emptyset = 1$ because Φ is group-like.

In [Dri91], Drinfel'd gives an explicit associator Φ_{KZ} over $\mathbb{C}$, known as the Drinfel'd associator and associated to a Knizhnik-Zamolodchikov equation (KZ equation). More precisely, consider the KZ equation (one can also see [Fur03][§3]).

$$\frac{\partial g}{\partial u} = \left(\frac{X_0}{u} + \frac{X_1}{u-1}\right) \cdot g(u) \tag{KZ}$$

where g is an analytic function in one complex variable u with values in $\mathbb{C}\langle\langle X_0, X_1\rangle\rangle$ (analytic means that each coefficient is an analytic function). This equation has singularities only at 0, 1 and ∞. The equation (KZ) has a unique solution on $C = \mathbb{C} \setminus (]-\infty, 0] \cup [1, \infty[)$ having a specified value at a given point in C, because C is simply connected. Moreover, at 0 (resp. 1), there exists a unique solution $g_0(u)$ (resp. $g_1(u)$) such that

$$g_0(u) \sim u^{X_0} \quad (u \to 0) \qquad \big(\text{resp. } g_1(u) \sim (1-u)^{X_1} \quad (u \to 1)\big).$$

As g_0 and g_1 are invertible with specified asymptotic behavior, they must coincide up to multiplication on the right by an invertible element in $\mathbb{C}\langle\langle X_0, X_1\rangle\rangle$.

Definition 1.5. The *Drinfel'd associator* [1] Φ_{KZ} is the element in $\mathbb{C}\langle\langle X_0, X_1\rangle\rangle$ defined by

$$g_0(u) = g_1(u)\Phi_{KZ}(X_0, X_1).$$

In [Dri91], Drinfel'd proved the following result.

Proposition 1.6. *The element Φ_{KZ} is a group-like element and it satisfies* (I), (II) *with $\mu = 2i\pi$, and* (III) *of definition 1.4. That is,*

$$\Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0) = 1 \tag{I$_{\mathrm{KZ}}$}$$

$$e^{i\pi X_0}\Phi_{KZ}(X_\infty, X_0)e^{i\pi X_\infty}\Phi_{KZ}(X_1, X_\infty)e^{i\pi X_1}\Phi_{KZ}(X_0, X_1) = 1 \quad \textit{with} \quad X_0 + X_1 + X_\infty = 0 \tag{II$_{\mathrm{KZ}}$}$$

$$\Phi_{KZ}(X_{12}, X_{23})\Phi_{KZ}(X_{34}, X_{45})\Phi_{KZ}(X_{51}, X_{12})\Phi_{KZ}(X_{23}, X_{34})\Phi_{KZ}(X_{45}, X_{51}) = 1 \quad \textit{in } U\mathfrak{B}_5. \tag{III$_{\mathrm{KZ}}$}$$

[1]In [Dri91], Drinfel'd actually defined ϕ_{KZ} rather than Φ_{KZ}, where $\phi_{KZ}(X_0, X_1) = \Phi_{KZ}(\frac{1}{2i\pi}X_0, \frac{1}{2i\pi}X_1)$ and is defined via the KZ equation $\frac{\partial g}{\partial u} = \frac{1}{2i\pi}\left(\frac{X_0}{u} + \frac{X_1}{u-1}\right) \cdot g(u)$.

1.2. **Multiple zeta values.** For a p-tuple $\mathbf{k} = (k_1, \ldots, k_p)$ of strictly positive integers with $k_1 \geqslant 2$, the multiple zeta value $\zeta(\mathbf{k})$ is defined as

$$\zeta(\mathbf{k}) = \sum_{n_1 > \ldots > n_p > 0} \frac{1}{n_1^{k_1} \cdots n_p^{k_p}}.$$

Definition 1.7. The depth of a p-tuple of integers $\mathbf{k} = (k_1, \ldots, k_p)$ is $dp(\mathbf{k}) = p$, and its weight $wt(\mathbf{k})$ is $wt(\mathbf{k}) = k_1 + \cdots + k_p$.

To the tuple of integers $\mathbf{k}$, with $n = wt(\mathbf{k})$, we associate the n-tuple $\overline{k}$ of 0 and 1 by:

$$\overline{k} = (\underbrace{0, \ldots, 0}_{k_1 - 1 \text{ times}}, 1, \ldots, \underbrace{0, \ldots, 0}_{k_p - 1 \text{ times}}, 1) = (\varepsilon_n, \ldots, \varepsilon_1)$$

and the word in $\{X_0, X_1\}^*$

$$X_{\varepsilon_n} \cdots X_{\varepsilon_1}.$$

This makes it possible to associate a multiple zeta value $\zeta(W)$ to each word W in $X_0\{X_0, X_1\}^* X_1$ (where W begins with X_0 and ends with X_1).

Following Kontsevich and Drinfel'd, one can write the multiple zeta values as a Chen iterated integral [Che73]

$$\zeta(\mathbf{k}) = \int_0^1 (-1)^p \frac{\mathrm{d}u}{u - \varepsilon_n} \circ \cdots \circ \frac{\mathrm{d}u}{u - \varepsilon_1}.$$

Note that, as $k_1 \geqslant 2$, we have $\varepsilon_n = 0$. This expression as an iterated integral leads directly to an expression of the multiple zeta values as an integral over a simplex

$$\zeta(\mathbf{k}) = \int_{\Delta_n} (-1)^p \frac{\mathrm{d}t_1}{t_1 - \varepsilon_1} \wedge \cdots \wedge \frac{\mathrm{d}t_n}{t_n - \varepsilon_n}$$

where $\Delta_n = \{0 < t_1 < \ldots < t_n < 1\}$.

Thanks to the work of Boutet-de-Monvelle, Ecalle, Gonzales-Lorca and Zagier, with the further developments by Ihara, Kaneko or Furusho, we can extend the definition of multiple zeta values to tuples without the condition $k_1 \geqslant 2$ (see [GL98], [Rac02], [IKZ06] or [Fur03]). These extended multiple zeta values are called regularized multiple zeta values, and we speak of regularizations. We will be interested in a specific regularization, the *shuffle regularization.*

Definition 1.8 (Shuffle product)**.** A shuffle of $\{1, 2, \ldots, n\}$ and $\{1, \ldots, m\}$ is a permutation σ of $\{1, 2, \ldots, n+m\}$ such that:

$$\sigma(1) < \sigma(2) < \cdots < \sigma(n) \qquad \text{and} \qquad \sigma(n+1) < \sigma(n+2) < \cdots < \sigma(n+m).$$

The set of all the shuffles of $\{1, 2, \ldots, n\}$ and $\{1, \ldots, m\}$ is denoted by $\mathrm{sh}(n, m)$

Let $V = X_{i_1} \cdots X_{i_n}$ and $W = X_{i_{n+1}} \cdots X_{i_{n+m}}$ be two words in $\mathcal{W}_{0,1}$. The shuffle of V and W is the collection of words

$$\mathrm{sh}(V, W) = (X_{i_{\sigma^{-1}(1)}} X_{i_{\sigma^{-1}(2)}} \cdots X_{i_{\sigma^{-1}(n+m)}})_{\sigma \in \mathrm{sh}(n,m)}.$$

Working in $\mathbb{C}\langle\langle X_0, X_1 \rangle\rangle$, we will also consider the sum

$$V ш W = \sum_{U \in \mathrm{sh}(V,W)} U = \sum_{\sigma \in \mathrm{sh}(n,m)} X_{i_{\sigma^{-1}(1)}} X_{i_{\sigma^{-1}(2)}} \cdots X_{i_{\sigma^{-1}(n+m)}}$$

and extend the shuffle product ш by linearity.

Definition 1.9. The *shuffle regularization* of the multiple zeta values is the collection of real numbers $\left(\zeta^{ш}(W)\right)_{W \in \mathcal{W}_{0,1}}$ such that:

(1) $\zeta^{ш}(X_0) = \zeta^{ш}(X_1) = 0$,
(2) $\zeta^{ш}(W) = \zeta(W)$ for all $W \in X_0 \mathcal{W}_{0,1} X_1$,

(3) $\zeta^{ш}(V)\zeta^{ш}(W) = \sum_{U \in \mathrm{sh}(V,W)} \zeta^{ш}(U)$ for all $V, W \in \mathcal{W}_{0,1}$

These regularized multiple zeta values $\zeta^{ш}(W)$, for W not in $X_0\mathcal{W}_{0,1}X_1$, are in fact linear combinations of the usual multiple zeta values, which were given explicitly by Furusho in [Fur03]. Seeing $\zeta^{ш}$ as a linear map from $\mathbb{C}\langle\langle X_0, X_1\rangle\rangle$ to $\mathbb{R}$, one can then rewrite the third condition as

$$\zeta^{ш}(V ш W) = \zeta^{ш}(V)\zeta^{ш}(W).$$

The coefficients of the Drinfel'd associator can be written in an explicit way using convergent multiple zeta values [Fur03].

Proposition 1.10. *Using the shuffle regularization we can write (*[LM96], [GL98], [Fur03]*)*

$$\Phi_{KZ}(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} (-1)^{dp(W)} \zeta^{ш}(W) W.$$

1.3. **Main results.** In Theorem 2.4 and Theorem 2.11 we will give explicit relations between the coefficients of the series defining an associator Φ equivalent to the relation (I) and (II) satisfied by Φ. Both were well-known, as it is easy to expand the product of the associators in $U\mathfrak{F}_2$, even if the author does not know whether the relations of Theorem 2.11 have actually appeared explicitly in the literature. In the case of the pentagon relation (III), writing down relations between the coefficients implies fixing a basis B of $U\mathfrak{B}_5$. Even if fixing such a basis breaks the natural symmetry of the pentagon relation (III), it makes it possible to give an explicit family of relations between the coefficients of Φ equivalent to ($\mathrm{III}_{\mathrm{KZ}}$). More precisely, decomposing a word W in the subset of letters $X_{34}, X_{45}, X_{24}, X_{12}, X_{23}$ in the basis B we have

$$W = \sum_{b \in B} l_{b,W} b,$$

and we obtain the following theorem.

Theorem (Theorem 2.15)**.** *The relation* (III) *is equivalent to the family of relations*

$$\forall b \in B \ (b \neq 1) \qquad \sum_{W \in \{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*} l_{b,W} C_{5,W} = 0,$$

where $C_{5,W}$ are explicitly given by:

$$C_{5,W} = \sum_{\substack{U_1, \ldots, U_5 \in \mathcal{W} \\ U_1 \cdots U_5 = W}} Z_{\rho_1(U_1)} Z_{\rho_2(U_2)} Z_{\rho_3(U_3)} Z_{\rho_4(U_4)} Z_{\rho_5(U_5)}.$$

In the above formula, $\mathcal{W}$ denotes $\{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*$ and the ρ_i are maps from $U\mathfrak{B}_5$ to $U\mathfrak{F}_2$ defined on the letters X_{12}, X_{23}, X_{34}, X_{45}, X_{24} in Definition 2.13 (as example: $\rho_1(X_{12}) = X_0$, $\rho_1(X_{23}) = X_1$ and $\rho_1(X_{34}) = \rho_1(X_{45}) = \rho_1(X_{24}) = 0$) with the convention that $Z_0 = 0$.

Applying this theorem to the particular basis B_4 coming from the identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{34}, X_{45}, X_{24}\rangle\rangle \rtimes k\langle\langle X_{12}, X_{23}\rangle\rangle,$$

one can compute the coefficients $l_{b,W}$ using the equation defining $U\mathfrak{B}_5$ (here $\rtimes$ denotes the complete semi-direct product). In particular it is easy to see that $l_{b,W}$ is in $\mathbb{Z}$ in that case. As shown by Ihara in the Lie algebra setting ([Iha90]), the above identification is induced by the morphism $f_4 : U\mathfrak{B}_5 \longrightarrow U\mathfrak{F}_2$ that sends X_{i4} to 0, X_{12} to X_0 and X_{23} to X_1 and by a particular choice of generators of the kernel (that is X_{24}, X_{34} and X_{45}).

After explaining each family of relations between the coefficients, we apply our results to the particular case of the Drinfel'd associator and give the corresponding family between multiple zeta values in equations (3), (9) and (14).

In Section 3 of the article, we explain how these families of relations between multiple zeta values are induced by iterated integrals on $\mathcal{M}_{0,4}$ and $\mathcal{M}_{0,5}$ using the bar construction studied by Brown in [Bro09]. The geometry of $\mathcal{M}_{0,5}$ allows us in Proposition 3.18 to interpret the coefficients $C_{5,W}$ using iterated integrals.

Proposition (Proposition 3.18)**.** *For any bar symbol ω_W dual to a word W in the letters X_{34}, X_{45}, X_{24}, X_{12}, X_{23}, we have*

$$C_{5,W} = \int_\gamma \mathrm{Reg}(\omega_W, \gamma)$$

where $\mathrm{Reg}(\omega, D)$ is the regularization of a bar symbol in $\oplus \mathrm{H}^1(\mathcal{M}_{0,5})^{\otimes n}$ along boundary components $D \subset \partial\mathcal{M}_{0,5}$ and where γ is a path around the standard cell of $\mathcal{M}_{0,5}(\mathbb{R})$.

This is a consequence of Theorem 3.16 which links the family of relations (14) to the bar construction.

Theorem (Theorem 3.16)**.** *The relation* ($\mathrm{III}_{\mathrm{KZ}}$) *is equivalent to the family of relations*

$$\forall b_4 \in B_4 \qquad \int_\gamma \mathrm{Reg}(b_4^*, \gamma) = 0$$

which is exactly the family of relations (14)*. Here $(b_4^*)_{b_4\in B_4}$ denotes the basis in $V(\mathcal{M}_{0,5})$, the bar construction on $\mathcal{M}_{0,5}$, dual to the basis B_4 of $U\mathfrak{B}_5$ described earlier.*

More generally, we then have that for any basis $F = (f)_{f\in F}$ on $V(\mathcal{M}_{0,5})$, the pentagon relation ($\mathrm{III}_{\mathrm{KZ}}$) is equivalent to

$$\forall f \in F \qquad \int_\gamma \mathrm{Reg}(f, \gamma) = 0.$$

Using different methods, and for another purpose, Brown, Gangl and Levin in [BGL10] obtain the same basis B_4^* of $V(\mathcal{M}_{0,5})$. In their work, the basis B_4^* is described using combinatorial objects. More precisely, they use maximal triangulations of rooted decorated polygons.

Instead of looking at all the elements of a basis F of $V(\mathcal{M}_{0,5})$, it is enough to consider only a subset of F that generates $V(\mathcal{M}_{0,5})$ as a shuffle algebra. Indeed, if ω in $V(\mathcal{M}_{0,5})$ is equal to $f_1 ш f_2$, the iterated integral $\int_\gamma \omega$ is equal to $\int_\gamma f_1 \int_\gamma f_2$. Thus it does not give a new relation between multiple zeta values. Considering a set of generators of the shuffle algebra leads to computing many less relations. In degrees 2 and 3 we have respectively 4 and 10 generators instead of 19 and 65 elements in the vector space basis. In the appendix, we will give these relations in degrees 2 and 3 using the basis B_4.

The multiplicative generators that we have found do not have a particularly simple expression in terms of symbols ω_W dual to words W in the letters X_{34}, X_{45}, X_{24}, X_{12}, X_{23}. But it seems to be linked with our particular choice of identification. Indeed, using X_{14}, X_{24} and X_{34} as generators of the kernel of $f_4 : U\mathfrak{B}_5 \longrightarrow U\mathfrak{F}_2$ leads to an other identification:

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{34}, X_{14}, X_{24}\rangle\rangle \rtimes k\langle\langle X_{12}, X_{23}\rangle\rangle$$

and to another basis $\tilde{B}_4$ of $U\mathfrak{B}_5$. Then, multiplicative generators can be found with a particularly simple expression in terms of symbols ω_W dual to words W in the

letters X_{34}, X_{14}, X_{24}, X_{12}, X_{23}. More precisely, writing such a word W as

$$W = \sum_{\tilde{b}_4 \in \tilde{B}_4} l_{\tilde{b}_4, W} \tilde{b}_4,$$

we can write $\tilde{b}_4^* = \sum_W l_{\tilde{b}_4, W} \omega_W$. The multiplicative generators in low degree are elements $\tilde{b}_4^*$ such that the number of $l_{\tilde{b}_4, W}$ is as minimal as possible. This seems to be a general fact.

2. Combinatorial description of associator relations

The goal of this section is, for any associator and for the particular case of Φ_{KZ}, to give an explicit expression for the relations between the coefficients derived from the associator relations (I), (II) and (III). For each of these relations, we will first study the case of a general associator and then deduce, for the Drinfel'd associator, relations between the regularized multiple zeta values. Let

$$\Phi = \sum_{W \in \mathcal{W}_{0,1}} Z_W W$$

be an associator. The idea will be to expand the product in the right hand side of the equations (I), (II) and (III) in a suitable basis of the space $U\mathfrak{F}_2$ or $U\mathfrak{B}_5$. Both $U\mathfrak{F}_2$ and $U\mathfrak{B}_5$ can be seen as a completion of polynomial algebras. Precisely, $U\mathfrak{F}_2$ is the completion of $k\langle X_0, X_1\rangle$, the polynomial algebra over k in two non-commutative variables, with respect to the ideal generated by X_0 and X_1. The algebra $U\mathfrak{B}_5$ is the completion with respect to the ideal generated by the X_{ij} of the polynomial algebra $k\langle X_{ij}\rangle/\mathcal{R}$ with $1 \leqslant i, j \leqslant 5$ and where $\mathcal{R}$ denotes the following relations:

- $X_{ii} = 0$ for $1 \leqslant i \leqslant 5$,
- $X_{ij} = X_{ji}$ for $1 \leqslant i, j \leqslant 5$,
- $\sum_{j=1}^{5} X_{ij} = 0$ for $1 \leqslant i \leqslant 5$,
- $[X_{ij}, X_{kl}] = 0$ if $\{i, j\} \cap \{k, l\} = \emptyset$.

Definition 2.1. A *basis* $B = (b)_{b \in B}$ of $U\mathfrak{F}_2$ (resp. $U\mathfrak{B}_5$) will denote a basis of the underlying vector space of the polynomial algebra $k\langle X_0, X_1\rangle$ (resp. $k\langle X_{ij}\rangle/\mathcal{R}$) such that

- Any element Ψ in $U\mathfrak{F}_2$ (resp. $U\mathfrak{B}_5$) can be uniquely written as a series
$$\Psi = \sum_{b \in B} a_b b.$$
- The elements b in B are homogeneous.

Speaking of a basis of $U\mathfrak{F}_2$ or $U\mathfrak{B}_5$, we will always mean a basis as in the above definition.

Remark 2.2. Let B be a basis (as above) of $U\mathfrak{F}_2$ (resp. $U\mathfrak{B}_5$). Assumptions in Definition 2.1 ensure that 1 is in B and

- Any W in $\mathcal{W}_{0,1}$ (resp. a word in the letters X_{ij}) can be uniquely written as
$$W = \sum_{b \in B} l_{b,W} b \qquad \text{in } U\mathfrak{F}_2 \quad (\text{resp. in } U\mathfrak{B}_5).$$
- Given such a decomposition for W, only finitely many $l_{b,W}$ are non zero when b runs through B.
- Fixing b, only finitely many $l_{b,W}$ are non zero when W runs through $\mathcal{W}_{0,1}$ (resp. runs through the words in the letters X_{ij}).

2.1. **The symmetry,** (I) **and** (I_{KZ})**.** Let P_2 be the product

$$P_2 = \Phi(X_0, X_1)\Phi(X_1, X_0).$$

As the monomials in $U\mathfrak{F}_2$, i.e. the words in $\mathcal{W}_{0,1}$, form a basis of $U\mathfrak{F}_2$, we can write P_2 as

$$P_2 = \sum_{W\in\mathcal{W}_{0,1}} C_{2,W} W = 1 + \sum_{W\in\mathcal{W}_{0,1},\, W\neq\emptyset} C_{2,W} W.$$

The relation (I) tells us that for each $W \in \mathcal{W}_{0,1}$, W being nonempty, we have

$$C_{2,W} = 0. \tag{1}$$

Example 2.3. In low degree we have the following relations:

- In degree one, there are just 2 words: X_0 and X_1 and (1) gives:
$$\begin{aligned} C_{2,X_0} &= Z_{X_0} + Z_{X_1} = 0 \\ C_{2,X_1} &= Z_{X_1} + Z_{X_0} = 0 \end{aligned}$$
- In degree two there are 4 words X_0X_0, X_0X_1, X_1X_0 and X_1X_1 and (1) gives:
$$\begin{aligned} C_{2,X_0X_0} &= Z_{X_0X_0} + Z_{X_0}Z_{X_1} + Z_{X_1X_1} = 0 \\ C_{2,X_0X_1} &= Z_{X_0X_1} + Z_{X_0}Z_{X_0} + Z_{X_1X_0} = 0 \\ C_{2,X_1X_0} &= Z_{X_1X_0} + Z_{X_1}Z_{X_1} + Z_{X_0X_1} = 0 \\ C_{2,X_0X_0} &= Z_{X_1X_1} + Z_{X_1}Z_{X_0} + Z_{X_0X_0} = 0 \end{aligned}$$
- In degree three there are 8 words. Looking at the coefficients of the words $X_0X_0X_1$ in P_2, equation (1) gives:
$$Z_{X_0X_0X_1} + Z_{X_0X_0}Z_{X_0} + Z_{X_0}Z_{X_1X_0} + Z_{X_1X_1X_0} = 0$$

Let θ be the automorphism of $U\mathfrak{F}_2$ that sends X_0 to X_1 and X_1 to X_0. Then we have:

Theorem 2.4. *The relation* (I) *is equivalent to the family of relations*

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}, \qquad \sum_{\substack{U_1,U_2\in\mathcal{W}_{0,1}\\ U_1U_2=W}} Z_{U_1}Z_{\theta(U_2)} = 0. \tag{2}$$

Proof. As $\Phi(X_1, X_0) = \theta(\Phi(X_0, X_1))$, we have

$$\begin{aligned} \Phi(X_1, X_0) = \theta\left(1 + \sum_{\substack{W\in\mathcal{W}_{0,1}\\ W\neq\emptyset}} Z_W W\right) &= 1 + \sum_{\substack{W\in\mathcal{W}_{0,1}\\ W\neq\emptyset}} Z_W \theta(W) \\ &= 1 + \sum_{\substack{W\in\mathcal{W}_{0,1}\\ W\neq\emptyset}} Z_{\theta(W)} W. \end{aligned}$$

Then, expanding the product P_2 and reorganizing, we have

$$\begin{aligned} \Phi(X_0, X_1)\Phi(X_1, X_0) &= \left(1 + \sum_{\substack{U_1\in\mathcal{W}_{0,1}\\ U_1\neq\emptyset}} Z_{U_1}U_1\right)\left(1 + \sum_{\substack{U_2\in\mathcal{W}_{0,1}\\ U_2\neq\emptyset}} Z_{\theta(U_2)}U_2\right) \\ &= 1 + \sum_{\substack{W\in\mathcal{W}_{0,1}\\ W\neq\emptyset}} \left(\sum_{\substack{U_1,U_2\in\mathcal{W}_{0,1}\\ U_1U_2=W}} Z_{U_1}Z_{\theta(U_2)}\right) W. \end{aligned}$$

□

Corollary 2.5. *The relation* (I_{KZ}) *is equivalent to the family of relations*

(3) $\forall W \in \mathcal{W}_{0,1},\ W \neq \emptyset,$

$$\sum_{\substack{U_1,U_2\in\mathcal{W}_{0,1}\\ U_1U_2=W}} (-1)^{dp(U_1)}\zeta^{\shuffle}(U_1)(-1)^{dp(\theta(U_2))}\zeta^{\shuffle}(\theta(U_2)) = 0,$$

that family being equivalent to the following

$$\forall W \in \mathcal{W}_{0,1},\ W \neq \emptyset, \qquad \sum_{\substack{U_1,U_2\in\mathcal{W}_{0,1}\\ U_1U_2=W}} (-1)^{|U_2|}\zeta^{\shuffle}(U_1)\zeta^{\shuffle}(\theta(U_2)) = 0. \tag{4}$$

Remark 2.6. If $W = X_{\varepsilon_1}\cdots X_{\varepsilon_n}$ is a word in $\mathcal{W}_{0,1}$, we define $\overleftarrow{W}$ to be the word $W = X_{\varepsilon_n}\cdots X_{\varepsilon_1}$. One can then check that the family of relations (3) (and thus (I_{KZ})) is implied by the following:

(1) *Shuffle relations*:

$$\text{for all } V \text{ and } W \text{ in } \mathcal{W}_{0,1}, \qquad \zeta^{\shuffle}(V \shuffle W) = \zeta^{\shuffle}(V)\zeta^{\shuffle}(W).$$

(2) *Duality relations* [Ohn99, Zag94]:

$$\text{for all } W \text{ in } \mathcal{W}_{0,1}, \qquad \zeta^{\shuffle}(W) = \zeta^{\shuffle}(\theta(\overleftarrow{W})).$$

The author does not know whether one can deduce the duality relations from the double shuffle relations.

The duality relations may be derived from (I_{KZ}), that is

$$\Phi_{KZ}(X_0,X_1)\Phi_{KZ}(X_1,X_0) = 1,$$

and correspond geometrically to a change of variables $t_i = 1 - u_i$ in the iterated integral representation of the multiple zeta values. In order to recover duality relations directly from (I) and the group-like property, the argument goes as follows. We want to show that a non-commutative power series in $U\mathfrak{F}_2$

$$\Phi(X_0,X_1) = 1 + \sum_{W\in\mathcal{W}_{0,1}\setminus\{\emptyset\}} C_W W$$

which is a group-like element and satisfies the 2-cycle equation

$$\Phi(X_0,X_1)\Phi(X_1,X_0) = 1$$

has coefficients that satisfy the duality relations

$$\forall W \in \mathcal{W}_{0,1}, \quad W \neq \emptyset, \qquad C_{\theta(\overleftarrow{W})} = (-1)^{wt(W)}C_W. \tag{5}$$

Applying this result to the Drinfel'd associator, that is for

$$C_W = (-1)^{dp(W)}\zeta^{\shuffle}(W),$$

one derives from (I_{KZ}) the duality relations for the multiple zeta values, that is

$$\forall W \in \mathcal{W}_{0,1}\setminus\{\emptyset\}, \qquad \zeta^{\shuffle}(W) = \zeta^{\shuffle}(\theta(\overleftarrow{W})).$$

To obtain the set of relations (5), one should first remark that

$$\begin{aligned}\Phi(X_0,X_1)^{-1} &= 1 + \sum_{W\in\mathcal{W}_{0,1}\setminus\{\emptyset\}} (-1)^{wt(W)}C_W\overleftarrow{W}\\ &= 1 + \sum_{W\in\mathcal{W}_{0,1}\setminus\{\emptyset\}} (-1)^{wt(\overleftarrow{W})}C_{\overleftarrow{W}}W.\end{aligned}$$

As the group elements are Zariski dense in the group-like elements, one has the above equality because the inverse of a group element $g = e^{\varepsilon_1 X_{i_1}} \cdots e^{\varepsilon_n X_{i_n}}$, with X_{i_k} in $\{X_0, X_1\}$ and ε_i in $\{\pm 1\}$, is given by $g^{-1} = e^{-\varepsilon_n X_{i_n}} \cdots e^{-\varepsilon_1 X_{i_1}}$. Then, as

$$\Phi(X_1, X_0) = 1 + \sum_{W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}} C_W \theta(W) = 1 + \sum_{W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}} C_{\theta(W)} W,$$

using the 2-cycle equation (I) written as $\Phi(X_1, X_0) = \Phi(X_0, X_1)^{-1}$, one obtains

$$\forall W \in \mathcal{W}_{0,1}, \quad W \neq \emptyset, \qquad C_{\theta(W)} = (-1)^{wt(\overleftarrow{W})} C_{\overleftarrow{W}}.$$

The above set of relations is equivalent to the duality relations (5).

2.2. **The 3-cycle or the hexagon relation,** (II) **and** ($\mathrm{II}_{\mathrm{KZ}}$)**.** For any element $P = \sum_{W \in \mathcal{W}_{0,1}} a_W W$ in $U\mathfrak{F}_2$, let $\mathrm{C}_{0,1}(P|W)$ be the coefficient a_W of the monomial W.

Let P_3 be the product

$$P_3 = e^{\frac{\mu}{2} X_0} \Phi(X_\infty, X_0) e^{\frac{\mu}{2} X_\infty} \Phi(X_1, X_\infty) e^{\frac{\mu}{2} X_1} \Phi(X_0, X_1).$$

We can write P_3 as

$$P_3 = \sum_{W \in \mathcal{W}_{0,1}} \mathrm{C}_{0,1}(P_3|W) W = \sum_{W \in \mathcal{W}_{0,1}} C_{3,W} W.$$

The relation (II) tells us that for each $W \in \mathcal{W}_{0,1}$, $W \neq \emptyset$, we have

$$C_{3,W} = 0. \tag{6}$$

In order to make these coefficients explicit, we will need some definitions.

Definition 2.7. Let α_0 (resp. α_1 and α_∞) be the endomorphism of $U\mathfrak{F}_2$ defined on X_0 and X_1 by:

$$\alpha_0(X_0) = X_0 \qquad \text{and} \qquad \alpha_0(X_1) = 0,$$

respectively

$$\alpha_1(X_0) = 0 \qquad \text{and} \qquad \alpha_1(X_1) = X_1$$

and

$$\alpha_\infty = -(\alpha_0 + \alpha_1).$$

Let $\tilde{\alpha}_i$ be the composition of α_i with $X_0, X_1 \mapsto 1$.

The following proposition is a consequence of the expression of the exponential

$$\forall P \in U\mathfrak{F}_2 \qquad \exp(P) = \sum_{n \geqslant 0} \frac{P^n}{n!}$$

and of the equality

$$(-X_0 - X_1)^n = \sum_{\substack{W \in \mathcal{W}_{0,1} \\ |W| = n}} (-1)^{|W|} W. \tag{7}$$

Proposition 2.8. *Let W be a word in $\mathcal{W}_{0,1}$. Then*

$$\mathrm{C}_{0,1}(e^{\frac{\mu}{2} X_0}|W) = \frac{\mu^{|W|}}{2^{|W|}|W|!} \tilde{\alpha}_0(W),$$

$$\mathrm{C}_{0,1}(e^{\frac{\mu}{2} X_1}|W) = \frac{\mu^{|W|}}{2^{|W|}|W|!} \tilde{\alpha}_1(W) \qquad \textit{and}$$

$$\mathrm{C}_{0,1}(e^{\frac{\mu}{2} X_\infty}|W) = (-1)^{|W|} \frac{\mu^{|W|}}{2^{|W|}|W|!}.$$

In order to describe the coefficient of $\Phi(X_i, X_j)$ with either one of the variables being X_∞, we introduce a set of different decompositions of W into sub-words.

Definition 2.9. Let W be a word in $\mathcal{W}_{0,1}$. For $i \in \{0,1\}$, let $\mathrm{dec}_{0,1}(W, X_i)$ be the set of tuples $(V_1, X_i^{k_1}, V_2, X_i^{k_2}, \dots, V_p, X_i^{k_p})$ with

(1) $1 \leqslant p < \infty$,
(2) $V_j \in \mathcal{W}_{0,1}$ and $V_2, \dots, V_p \neq \emptyset$,
(3) $k_1, \dots, k_{p-1} > 0$ and $k_p \geqslant 0$

such that

$$W = V_1 X_i^{k_1} V_2 X_i^{k_2} \cdots V_p X_i^{k_p}.$$

We will write $(\mathbf{V}, \mathbf{k}) \in \mathrm{dec}_{0,1}(W, X_i)$ instead of

$$(V_1, X_i^{k_1}, V_2, X_i^{k_2}, \dots, V_p, X_i^{k_p}) \in \mathrm{dec}_{0,1}(W, X_i)$$

and $|\mathbf{V}|$ (resp. $|\mathbf{k}||$) will denote $|V_1| + \cdots + |V_p|$ (resp. $k_1 + \cdots + k_p$).

The following proposition describes the coefficient of W in the series $\Phi(X_0, X_1)$, $\Phi(X_\infty, X_0)$ and $\Phi(X_1, X_\infty)$.

Proposition 2.10. *Let W be a word in $\mathcal{W}_{0,1}$. We have*

$$\mathrm{C}_{0,1}(\Phi(X_0, X_1)|W) = Z_W.$$

The coefficients $\mathrm{C}_{0,1}(\Phi(X_\infty, X_0)|W)$ and $\mathrm{C}_{0,1}(\Phi(X_1, X_\infty)|W)$ can be written as

$$\mathrm{C}_{0,1}(\Phi(X_\infty, X_0)|W) = \sum_{(\mathbf{V},\mathbf{k}) \in \mathrm{dec}_{0,1}(W, X_0)} (-1)^{|\mathbf{V}|} Z_{X_0^{|V_1|} X_1^{k_1} X_0^{|V_2|} X_1^{k_2} \cdots X_0^{|V_p|} X_1^{k_p}}$$

and

$$\mathrm{C}_{0,1}(\Phi(X_1, X_\infty)|W) = \sum_{(\mathbf{V},\mathbf{k}) \in \mathrm{dec}_{0,1}(W, X_1)} (-1)^{|\mathbf{V}|} Z_{X_1^{|V_1|} X_0^{k_1} X_1^{|V_2|} X_0^{k_2} \cdots X_1^{|V_p|} X_0^{k_p}}.$$

Proof. The first statement is immediate. Let $\mathcal{L}_{2,c}(\mathbb{N})$ denote the set of double p-tuples ($0 \leqslant p < \infty$) of integers $((l_1, \dots, l_p), (k_1, \dots k_p))$ with $k_i, l_i \in \mathbb{N}$, such that, when $p \geqslant 2$ one has $k_i > 0$ for $i = 1, \dots, p-1$, and $l_j > 0$ for $j = 2, \dots, p$. Let $(\mathbf{l}, \mathbf{k})$ denote an element of $\mathcal{L}_{2,c}(\mathbb{N})$. We can write $\Phi(X_\infty, X_0)$ as

$$\Phi(X_\infty, X_0) = \sum_{(\mathbf{l},\mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \cdots X_0^{l_p} X_1^{k_p}} X_\infty^{l_1} X_0^{k_1} \cdots X_\infty^{l_p} X_0^{k_p}$$

which equals

$$\sum_{(\mathbf{l},\mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \cdots X_0^{l_p} X_1^{k_p}} (-1)^{|\mathbf{l}|} (X_0 + X_1)^{l_1} X_0^{k_1} \cdots (X_0 + X_1)^{l_p} X_0^{k_p}.$$

Reorganizing, we see that the expression of $\mathrm{C}_{0,1}(\Phi(X_\infty, X_0)|W)$ follows from (7); the case of $\mathrm{C}_{0,1}(\Phi(X_1, X_\infty)|W)$ is identical. $\square$

Theorem 2.11. *The relation* (II) *is equivalent to the family of relations*

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}, \tag{8}$$

$$\sum_{\substack{W_1,\dots,W_6 \in \mathcal{W}_{0,1}\\ W_1\cdots W_6 = W}} \frac{\mu^{|W_1|}}{2^{|W_1|}|W_1|!}\tilde{\alpha_0}(W_1)\times$$
$$\left(\sum_{\substack{(\mathbf{U},\mathbf{k})\in\\ \mathrm{dec}_{0,1}(W_2,X_0)}} (-1)^{|\mathbf{U}|} Z_{X_0^{|U_1|}X_1^{k_1}\cdots X_0^{|U_p|}X_1^{k_p}}\right)(-1)^{|W_3|}\frac{\mu^{|W_3|}}{2^{|W_3|}|W_3|!}\times$$
$$\left(\sum_{\substack{(\mathbf{V},\mathbf{l})\in\\ \mathrm{dec}_{0,1}(W_4,X_1)}} (-1)^{|\mathbf{V}|} Z_{X_1^{|V_1|}X_0^{l_1}\cdots X_1^{|V_p|}X_0^{l_p}}\right)\frac{\mu^{|W_5|}}{2^{|W_5|}|W_5|!}\tilde{\alpha_1}(W_5)Z_{W_6} = 0.$$

Proof. The relation (II) is equivalent to the family of relations

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\} \qquad \mathrm{C}_{0,1}(P_3, W) = 0.$$

As P_3 is a product of six factors, this is equivalent to

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}$$
$$\sum_{\substack{W_1,\dots,W_6 \in \mathcal{W}_{0,1}\\ W_1\cdots W_6 = W}} \mathrm{C}_{0,1}(e^{\frac{\mu}{2}X_0}, W_1)\mathrm{C}_{0,1}(\Phi(X_\infty, X_0), W_2)\cdot$$
$$\mathrm{C}_{0,1}(e^{\frac{\mu}{2}X_\infty}, W_3)\mathrm{C}_{0,1}(\Phi(X_1, X_\infty), W_4)\cdot$$
$$\mathrm{C}_{0,1}(e^{\frac{\mu}{2}X_1}, W_5)\mathrm{C}_{0,1}(\Phi(X_0, X_1), W_6) = 0.$$

The proposition then follows from Proposition 2.8 and 2.10. □

Corollary 2.12. *The relation* ($\mathrm{II}_{\mathrm{KZ}}$) *is equivalent to the family of relations*

$$\forall W \in \mathcal{W}_{0,1} \setminus \{\emptyset\}, \tag{9}$$

$$\sum_{\substack{W_1,\dots,W_6 \in \mathcal{W}_{0,1}\\ W_1\cdots W_6 = W}} \frac{(i\pi)^{|W_1|}}{|W_1|!}\tilde{\alpha_0}(W_1)\times$$
$$\left(\sum_{\substack{(\mathbf{U},\mathbf{k})\\ \in \mathrm{dec}_{0,1}(W_2,X_0)}} (-1)^{|W_2|}\zeta^{ш}(X_0^{|U_1|}X_1^{k_1}\cdots X_0^{|U_p|}X_1^{k_p})\right)(-1)^{|W_3|}\frac{(i\pi)^{|W_3|}}{|W_3|!}\times$$
$$\left(\sum_{\substack{(\mathbf{V},\mathbf{l})\\ \in \mathrm{dec}_{0,1}(W_4,X_1)}} \zeta^{ш}(X_1^{|V_1|}X_0^{l_1}\cdots X_1^{|V_p|}X_0^{l_p})\right)\frac{(i\pi)^{|W_5|}}{|W_5|!}\tilde{\alpha_1}(W_5)\times$$
$$(-1)^{dp(W_6)}\zeta^{ш}(W_6) = 0.$$

2.3. **The 5-cycle or the pentagon relation,** (III) **and** ($\mathrm{III}_{\mathrm{KZ}}$)**.** In order to find families of relations between the coefficients equivalent to (I) and (II), we decomposed the product P_2 and P_3 in the basis of $U\mathfrak{F}_2$ given by the words in X_0 and X_1. We will do the same thing here; however, the monomials in the variables X_{ij} do not form a basis of $U\mathfrak{B}_5$, because there are relations between the X_{ij}. Using

the defining relations of $U\mathfrak{B}_5$, we see that $X_{51} = -X_{12} - X_{13} - X_{14}$, and that

$$\begin{aligned} X_{51} &= -X_{54} - X_{53} - X_{52} \\ &= 2X_{23} + 2X_{24} + 2X_{34} + X_{12} + X_{13} + X_{14}. \end{aligned}$$

Then, as the characteristic of k is zero, we have $X_{51} = X_{23} + X_{24} + X_{34}$. In this section, we will expand the product in the R.H.S of III using this relation and then decompose this product in a basis of $U\mathfrak{B}_5$. Let B denote a basis of $U\mathfrak{B}_5$ (in the sense of Definition 2.1), and let B_4 denote the basis of $U\mathfrak{B}_5$ coming from the identification

$$U\mathfrak{B}_5 \simeq k\langle\langle X_{24}, X_{34}, X_{45}\rangle\rangle \rtimes k\langle\langle X_{12}, X_{23}\rangle\rangle.$$

This identification is induced by the morphism $f_4 : U\mathfrak{B}_5 \longrightarrow U\mathfrak{F}_2$ that maps X_{i4} to 0 ($1 \leqslant i \leqslant 5$), X_{12} to X_0, X_{23} to X_1; the images of the other generators are easily deduced from these, by the choice of X_{24}, X_{34} and X_{45} as generators of the kernel of f_4 (see [Iha90]). Using the relation defining $U\mathfrak{B}_5$, one sees that

$$[X_{ij}, X_{jk}] = -[X_{ik}, X_{jk}] \qquad i \neq j, k \text{ and } j \neq k$$

which gives for example

$$[X_{12}, X_{24}] = -[X_{14}, X_{24}] = [X_{34}, X_{24}] + [X_{45}, X_{24}].$$

The basis B_4 is formed by 1 and the monomials, that is words of the form $U_{245}V_{123}$ where U_{245} is a word in ${}_{24}\mathcal{W}_{34,45} = \{X_{24}, X_{34}, X_{45}\}^*$ and V_{123} is in $\mathcal{W}^{12,23} = \{X_{12}, X_{23}\}^*$. Speaking of the empty word $\emptyset$ in B_4, we will mean 1 when seen in $U\mathfrak{B}_5$ and $\emptyset$ when seen as the word.

Let $\mathcal{W}$ be the dictionary $\{X_{24}, X_{34}, X_{45}, X_{12}, X_{23}\}^*$, and let ${}_{24}\mathcal{W}_{34}^{23}$ and ${}_{24}\mathcal{W}_{34}^{12,23}$ be respectively the sub-dictionary

$${}_{24}\mathcal{W}_{34}^{23} = \{X_{23}, X_{24}, X_{34}\}^* \qquad \text{and} \qquad {}_{24}\mathcal{W}_{34}^{12,23} = \{X_{12}, X_{23}, X_{24}, X_{34}\}^*.$$

Let P_5 be the product in $U\mathfrak{B}_5$.

$$\Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{51}, X_{12})\Phi(X_{23}, X_{34})\Phi(X_{45}, X_{51}).$$

As $X_{51} = X_{23} + X_{24} + X_{34}$, we can write P_5 without using X_{51}

$$\begin{aligned} P_5 = \Phi(X_{12}, X_{23})\Phi(X_{34}, X_{45})\Phi(X_{23} + X_{24} + X_{34}, X_{12})\Phi(X_{23}, X_{34}) \\ \Phi(X_{45}, X_{23} + X_{24} + X_{34}). \end{aligned}$$

Expanding the terms $(X_{23} + X_{24} + X_{34})^n$ as

$$\sum_{\substack{W \in {}_{24}\mathcal{W}_{34}^{23} \\ |W| = n}} W,$$

we have

$$P_5 = \sum_{W \in \mathcal{W}} C_{5,W} W. \tag{10}$$

Despite the fact that this expression is not unique as a decomposition of P_5 in $\mathcal{W}$, these $C_{5,W}$ are the coefficients of a word W just after expanding the product P_5 without X_{51} (that is replacing X_{51} by $X_{23} + X_{24} + X_{34}$), and as such, they are unique and well defined.

Definition 2.13. Let ρ_1, ρ_2, ρ_3, ρ_4, ρ_5 be the morphisms from $U\mathfrak{B}_5$ to $U\mathfrak{F}_2$ defined respectively on the monomial X_{12}, X_{23}, X_{34}, X_{45}, X_{24} by:

$$\begin{array}{lllll}
\rho_1(X_{12}) = X_0, & \rho_1(X_{23}) = X_1, & \rho_1(X_{34}) = 0, & \rho_1(X_{45}) = 0, & \rho_1(X_{24}) = 0,\\
\rho_2(X_{12}) = 0, & \rho_2(X_{23}) = 0, & \rho_2(X_{34}) = X_0, & \rho_2(X_{45}) = X_1, & \rho_2(X_{24}) = 0,\\
\rho_3(X_{12}) = X_1, & \rho_3(X_{23}) = X_0, & \rho_3(X_{34}) = X_0, & \rho_3(X_{45}) = 0, & \rho_3(X_{24}) = X_0,\\
\rho_4(X_{12}) = 0, & \rho_4(X_{23}) = X_0, & \rho_4(X_{34}) = X_1, & \rho_4(X_{45}) = 0, & \rho_4(X_{24}) = 0,\\
\rho_5(X_{12}) = 0, & \rho_5(X_{23}) = X_1, & \rho_5(X_{34}) = X_1, & \rho_5(X_{45}) = X_0, & \rho_5(X_{24}) = X_1.
\end{array}$$

By convention, we will have $\rho_i(1) = \rho_i(\emptyset) = 1$.

Proposition 2.14. *For all words $W \in \mathcal{W}$ ($W \neq \emptyset$), the coefficient $C_{5,W}$ is given by*

$$C_{5,W} = \sum_{\substack{U_1,\dots,U_5 \in \mathcal{W}\\ U_1\cdots U_5 = W}} Z_{\rho_1(U_1)} Z_{\rho_2(U_2)} Z_{\rho_3(U_3)} Z_{\rho_4(U_4)} Z_{\rho_5(U_5)}, \tag{11}$$

where by convention $Z_0 = 0$ and $Z_1 = Z_\emptyset = 1$.

Proof. It is enough to show that the i-th factor of P_5 without using X_{51} can be written as

$$\sum_{U_i \in \mathcal{W}} Z_{\rho_i(U_i)} U_i.$$

As the first, second and fourth factors are similar, we will discuss only the first one. It is clear in the case of $\Phi(X_{12}, X_{23})$ that either U_1 is in $\mathcal{W}^{12,23}$ and its coefficient is then $Z_{\rho_1(U_1)}$, or U_1 is not in $\mathcal{W}^{12,23}$ and it does not appear in $\Phi(X_{12}, X_{23})$ which means that its coefficient is 0.

The third and fifth factors are similar and thus we will treat only the former. We can write $\Phi(X_{23} + X_{24} + X_{34}, X_{12})$ as

$$\sum_{(\mathbf{l},\mathbf{k}) \in \mathcal{L}_{2,c}(\mathbb{N})} Z_{X_0^{l_1} X_1^{k_1} \cdots X_0^{l_p} X_1^{k_p}} (X_{23} + X_{24} + X_{34})^{l_1} X_{12}^{k_1} \cdots (X_{23} + X_{24} + X_{34})^{l_p} X_{12}^{k_p}.$$

We can rewrite the previous sum as running over all the words in the letters X_{12}, X_{23}, X_{24} and X_{34} because $(X_{23} + X_{24} + X_{34})^l$ is equal to

$$\sum_{\substack{W \in {}_{24}\mathcal{W}_{34}^{23}\\ |W| = l}} W.$$

Using the unique decomposition (as word) of $U_3 \in {}_{24}\mathcal{W}_{34}^{12,23}$ as

$$U_3 = V_1 X_{12}^{k_1} \cdots V_p X_{12}^{k_p} \qquad \text{with } V_i \in {}_{24}\mathcal{W}_{34}^{23},$$

we see that each word U_3 in ${}_{24}\mathcal{W}_{34}^{12,23}$ appears one and only one time in $\Phi(X_{23} + X_{24} + X_{34}, X_{12})$ with the coefficient $Z_{X_0^{|V_1|} X_1^{k_1} \cdots X_0^{|V_p|} X_1}$. We finally have

$$\Phi(X_{23} + X_{24} + X_{34}, X_{12}) = \sum_{U_3 \in \mathcal{W}} Z_{\rho_3(U_3)} U_3.$$

$\square$

We fix a basis B of $U\mathfrak{B}_5$ (in the sense of Definition 2.1). Remark 2.2 ensures that for every W in $\mathcal{W}$, there exists a unique decomposition of W (in $U\mathfrak{B}_5$) in terms of linear combinations of elements of B

$$W = \sum_{b \in B} l_{b,W}\, b \qquad l_{b,W} \in k.$$

Then, using the basis B, we can find a family of relations equivalent to (III).

Theorem 2.15. *The relation* (III) *is equivalent to the family of relations*

$$(12)\quad \forall b \in B\ (b \neq 1) \qquad \sum_{W\in\mathcal{W}} l_{b,W} C_{5,W} = 0$$

where $C_{5,W}$ are given by Proposition 2.14.

Proof. As observed in Remark 2.2, for a given W in $\mathcal{W}$ there are only finitely many $l_{b,W}$ that are non zero. Moreover, for any b in B there are only finitely many $l_{b,W}$ that are non zero.

The product P_5 is then equal to

$$\begin{aligned} P_5 &= \sum_{W\in\mathcal{W}} C_{5,W} W \\ &= \sum_{W\in\mathcal{W}} C_{5,W} \left(\sum_{b\in B} l_{b,W} b\right) \\ &= \sum_{b\in B} \left(\sum_{W\in\mathcal{W}} l_{b,W} C_{5,W}\right) b. \end{aligned}$$

The relation (III) tells us that

$$P_5 = 1$$

which, because 1 is in B, means that $C_{5,\emptyset} = 1$ and

$$\forall b \in B\ (b \neq 1) \qquad \sum_{W\in\mathcal{W}} l_{b,W} C_{5,W} = 0.$$

□

Using the more common basis B_4 we have:

Corollary 2.16. *The relation* (III) *is equivalent to the family of relations*

$$(13)\quad \forall b_4 \in B_4\ (b_4 \neq 1) \qquad \sum_{W\in\mathcal{W}} l_{b_4,W} C_{5,W} = 0$$

where the $C_{5,W}$ are given by Proposition 2.14.

Remark 2.17. In the case of the basis B_4 one can check that the coefficients $l_{b_4,W}$ are in $\mathbb{Z}$.

The previous corollary, applied to the particular case of the Drinfel'd associator and making explicit the $C_{5,W}$ in terms of multiple zeta values, gives:

Theorem 2.18. *With the convention that $\zeta^{ш}(0) = 0$, the relation* ($\mathrm{III}_{\mathrm{KZ}}$) *is equivalent to the family of relations*

$$(14)\quad \forall b_4 \in B_4\ (b_4 \neq 1)$$
$$\sum_{W} l_{b_4,W} \left(\sum_{U_1\cdots U_5 = W} (-1)^{dp_1(U_1)+dp_2(U_2)+dp_3(U_3)+dp_4(U_4)+dp_5(U_5)} \right.$$
$$\left. \zeta^{ш}(\rho_1(U_1))\zeta^{ш}(\rho_2(U_2))\zeta^{ш}(\rho_3(U_3)\zeta^{ш}(\rho_4(U_4))\zeta^{ш}(\rho_5(U_5)) \right) = 0$$

where $dp_i(U)$ is the depth of $\rho_i(U)$ and the words W, U_i are in $\mathcal{W}$.

3. Bar Construction and associator relations

In this section, we suppose that k is $\mathbb{C}$. We review the notion of bar construction and its links with multiple zeta values. Those results have been shown in greater generality in [Che73] and [Bro09]. We will recall Brown's variant of Chen's reduced bar construction in the case of the moduli spaces of curves of genus 0 with 4 and 5 marked points, $\mathcal{M}_{0,4}$ and $\mathcal{M}_{0,5}$.

3.1. **Bar Construction.** The moduli space of curves of genus 0 with 4 marked points, $\mathcal{M}_{0,4}$, is

$$\mathcal{M}_{0,4} = \{(z_1, \dots, z_4) \in (\mathbb{P}^1)^4 \mid z_i \neq z_j \text{ if } i \neq j\} / \operatorname{PGL}_2(k)$$

and is identified as

$$\mathcal{M}_{0,4} \simeq \{t \in (\mathbb{P}^1) \mid t \neq 0, 1, \infty\}$$

by sending the point $[(0, t, 1, \infty)] \in \mathcal{M}_{0,4}$ to t.

The moduli space of curves of genus 0 with 5 marked points, $\mathcal{M}_{0,5}$, is

$$\mathcal{M}_{0,5} = \{(z_1, \dots, z_5) \in (\mathbb{P}^1)^5 \mid z_i \neq z_j \text{ if } i \neq j\} / \operatorname{PGL}_2(k)$$

and is identified as

$$\mathcal{M}_{0,5} \simeq \{(x, y) \in (\mathbb{P}^1)^2 \mid x, y \neq 0, 1, \infty \text{ and } x \neq y\}$$

by sending the point $[(0, xy, y, 1, \infty)] \in \mathcal{M}_{0,5}$ to (x, y). This identification can be interpreted as the composition of

$$\begin{array}{ccc} \mathcal{M}_{0,5} & \longrightarrow & \mathcal{M}_{0,4} \times \mathcal{M}_{0,4} \\ [(z_1, \dots, z_5)] & \longmapsto & [(z_1, z_2, z_3, z_5)] \times [(z_1, z_3, z_4, z_5)] \end{array}$$

with the previous identification of $\mathcal{M}_{0,4}$ using the fact that

$$[(0, xy, y, \infty)] = [(0, x, 1, \infty)].$$

For $\mathcal{M} = \mathcal{M}_{0,4}$ or $\mathcal{M} = \mathcal{M}_{0,5}$, Brown has defined in [Bro09] a graded Hopf k-algebra

$$V(\mathcal{M}) = \oplus_{m=0}^{\infty} V_m(\mathcal{M}) \subset \oplus_{m=0}^{\infty} \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})^{\otimes m}. \tag{15}$$

Here $V_0(\mathcal{M}) = k$, $V_1(\mathcal{M}) = \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})$ and $V_m(\mathcal{M})$ is the intersection of the kernel $\wedge_i$ for $1 \leqslant i \leqslant m-1$:

$$\begin{array}{ccc} \wedge_i : \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})^{\otimes m} & \longrightarrow & \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})^{\otimes m-i-1} \otimes \mathrm{H}^2_{\mathrm{DR}}(\mathcal{M}) \otimes \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})^{\otimes i-1} \\ \nu_m \otimes \cdots \otimes \nu_1 & \longmapsto & \nu_m \otimes \cdots \otimes (\nu_{i+1} \wedge \nu_i) \otimes \cdots \otimes \nu_1. \end{array}$$

Suppose that $\omega_1, \dots, \omega_k$ form a basis of $\mathrm{H}^1_{\mathrm{DR}}(\mathcal{M})$; then the elements of $V_m(\mathcal{M})$ can be written as linear combinations of symbols

$$\sum_{I=(i_1,\dots,i_m)} c_I [\omega_{i_m} | \dots | \omega_{i_1}],$$

with $c_I \in k$, which satisfy the integrability condition

$$\sum_{I=(i_1,\dots,i_m)} c_I \omega_{i_m} \otimes \cdots \otimes \omega_{i_{j+2}} \otimes (\omega_{i_{j+1}} \wedge \omega_{i_j}) \otimes \omega_{i_{j-1}} \otimes \cdots \otimes \omega_{i_1} = 0 \tag{16}$$

for all $1 \leqslant j \leqslant m-1$.

Definition 3.1. Brown's bar construction over $\mathcal{M}$ is the tensor product

$$B(\mathcal{M}) = \mathcal{O}_{\mathcal{M}} \otimes V(\mathcal{M}).$$

Theorem 3.2 ([Bro09]). *The bar construction $B(\mathcal{M})$ is a commutative graded Hopf algebra isomorphic to the 0^{Th} cohomology group of Chen's reduced bar complex on $\mathcal{O}_{\mathcal{M}}$:*

$$B(\mathcal{M}) \simeq \mathrm{H}^0(B(\Omega^\bullet \mathcal{O}_{\mathcal{M}})).$$

Let $\nu_m, \ldots, \nu_1$ be m holomorphic 1-forms in $\Omega^1(\mathcal{M})$. The iterated integral of the word $\nu_m \cdots \nu_1$, denoted by

$$\int \nu_m \circ \cdots \circ \nu_1,$$

is the application that sends any path $\gamma : [0,1] \to \mathcal{M}$ to

$$\int_\gamma \nu_m \circ \cdots \circ \nu_1 = \int_{0<t_1<\ldots<t_m} \gamma^* \nu_1(t_1) \wedge \cdots \wedge \gamma^* \nu_m(t_m).$$

This value is called the iterated integral of $\nu_m \cdots \nu_1$ along γ. We extend these definitions by linearity to linear combinations of forms $\sum_I c_I \nu_{i_m} \ldots \nu_{i_1}$.

When, for any γ, the iterated integral

$$\int_\gamma \sum_I c_I \nu_m \circ \cdots \circ \nu_1$$

depends only on the homotopy class of γ, we say it is an homotopy invariant iterated integral and denote it by $\int \sum c_I \nu_m \circ \cdots \circ \nu_1$. Let $L(\mathcal{M})$ denote the set of all homotopy invariant iterated integrals.

Proposition 3.3 ([Bro09]). *The morphism ρ defined by*

$$\begin{array}{ccc} \rho : B(\mathcal{M}) & \longrightarrow & L(\mathcal{M}) \\ \sum_I c_I [\omega_{i_m} | \cdots | \omega_{i_1}] & \longmapsto & \int \sum_I c_I \omega_{i_m} \circ \cdots \circ \omega_{i_1} \end{array}$$

is an isomorphism.

Remark 3.4. In particular for any such γ homotopically equivalent to zero, we have for all $\sum_I c_I [\omega_{i_m} | \cdots | \omega_{i_1}]$ in $V(\mathcal{M})$:

$$\sum_I c_I \int_\gamma \omega_{i_m} \circ \cdots \circ \omega_{i_1} = 0$$

3.2. **Bar Construction on $\mathcal{M}_{0,4}$, symmetry and hexagon relations.** Here, we will show how the symmetry relations (I_{KZ}) and the hexagon ($\mathrm{II}_{\mathrm{KZ}}$) relations are related to the bar construction on $\mathcal{M}_{0,4}$.

First of all we should remark that $B(\mathcal{M}_{0,4})$ is extremely simple.

Proposition 3.5. *Let ω_0 and ω_1 denote respectively the differential 1-form, in $\Omega^1(\mathcal{M}_{0,4})$, $\frac{\mathrm{d}t}{t}$ and $\frac{\mathrm{d}t}{t-1}$.*

Then, any element $[\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$ with ε_i in $\{0,1\}$ is an element of $V(\mathcal{M}_{0,4})$. Moreover, the family of these elements is a basis of $V(\mathcal{M}_{0,4})$.

Proof. As $\omega_0 \wedge \omega_1 = 0$, the integrability condition (16) is automatically satisfied, so any element $[\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$ ($\varepsilon_i = 0, 1$) is an element of $V(\mathcal{M}_{0,4})$. Moreover, as (ω_0, ω_1) is a basis of $\mathrm{H}^1_{\mathrm{DR}}(\mathcal{M}_{0,4})$, the elements $[\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$ form a basis of $V(\mathcal{M}_{0,4})$. □

Sending X_0 to ω_0 and X_1 to ω_1 gives a one to one correspondence between words $W = X_{\varepsilon_n} \cdots X_{\varepsilon_1}$ in $\mathcal{W}_{0,1}$ and the elements $[\omega_{\varepsilon_n} | \cdots | \omega_{\varepsilon_1}]$ of the previous basis of $V(\mathcal{M}_{0,4})$. This correspondence allows us to identify $V(\mathcal{M}_{0,4})$ with the graded dual of $U\mathfrak{F}_2$,

$$V(\mathcal{M}_{0,4}) \simeq (U\mathfrak{F}_2)^*.$$

The word $W = X_{\varepsilon_n} \cdots X_{\varepsilon_1}$ is sent to its dual $W^* = \omega_W = [\omega_{\varepsilon_n}|\cdots|\omega_{\varepsilon_1}]$.

Remark 3.6. Let α and β be two paths in a variety with $\alpha(1) = \beta(0)$. We will denote by $\beta \circ \alpha$ the composed path beginning with α and ending with β.

The iterated integral of $\omega = \omega_n \cdots \omega_1$ along $\beta \circ \alpha$ is then equal to

$$\sum_{k=0}^{n} \left(\int_\beta \omega_n \circ \cdots \circ \omega_{n-k+1} \right) \left(\int_\alpha \omega_{n-k} \circ \cdots \circ \omega_1 \right). \tag{17}$$

Following [Bro09] and considering the three dihedral structures on $\mathcal{M}_{0,4}$, one can define 6 tangential base points: $\vec{01}$, $\vec{10}$, $\vec{1\infty}$, $\vec{\infty 1}$,$\vec{\infty 0}$ and $\vec{0\infty}$. Let p denote the path beginning at the tangential base point $\vec{01}$ and ending at $\vec{10}$ defined by $t \mapsto t$ and let p^{-1} denote its inverse $t \mapsto 1-t$.

If γ is a path, starting at a tangential base point $\vec{P}$ (and/or ending at a tangential base point $\vec{P'}$) an iterated integral $\int \omega$ may be divergent. However, one can give (as in [Bro09]) a value to that divergent integral; we speak of the regularized iterated integral.

If W is a word in $X_0\mathcal{W}_{0,1}X_1$, the iterated integral $\int_p \omega_W$ is convergent and is equal to $(-1)^{dp(W)}\zeta(W)$. If W is a word beginning by X_1 and/or ending by X_0 (that is in $\mathcal{W}_{0,1} \setminus X_0\mathcal{W}_{0,1}X_1$), then the regularized iterated integral $\int_p \omega_W$ is equal to $(-1)^{dp(W)}\zeta^{ш}(W)$.

We may, thereafter, omit the term *regularized* in the expressions "regularized iterated integral" or "regularized homotopy invariant iterated integral".

Theorem 3.7. *The relation* $(\mathrm{I}_{\mathrm{KZ}})$ *is equivalent to the family of relations*

$$\forall W \in \mathcal{W}_{0,1} \qquad \int_{p \circ p^{-1}} \omega_W = 0,$$

which is exactly the family (3).

Proof. Considering the KZ equation (KZ)

$$\frac{\partial g}{\partial u} = \left(\frac{X_0}{u} + \frac{X_1}{u-1} \right) \cdot g(u)$$

and the two normalized solutions at 0 and 1, g_0 and g_1, $\Phi_{KZ}(X_0, X_1)$ is the unique element in $U\mathfrak{F}_2$ such that

$$g_0(u) = g_1(u)\Phi_{KZ}(X_0, X_1).$$

Using the symmetry of the situation we also have

$$g_1(u) = g_0(u)\Phi_{KZ}(X_1, X_0).$$

The equation $(\mathrm{I}_{\mathrm{KZ}})$ comes from the uniqueness of such a solution normalized at 1:

$$g_1(u) = g_1(u)\Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0). \tag{18}$$

The elements $\Phi_{KZ}(X_0, X_1)$ and $\Phi_{KZ}(X_1, X_0)$ can be expressed using regularized iterated integrals as

$$\Phi_{KZ}(X_0, X_1) = \sum_{W \in \mathcal{W}_{0,1}} \left(\int_p \omega_W \right) W$$

and

$$\Phi_{KZ}(X_1, X_0) = \sum_{W \in \mathcal{W}_{0,1}} \left(\int_{p^{-1}} \omega_W \right) W.$$

Equation (18) corresponds to the comparison of the normalized solution g_1 with the solution given by analytic continuation of g_1 along $p \circ p^{-1}$. The product

$$\Phi_{KZ}(X_0, X_1)\Phi_{KZ}(X_1, X_0)$$

is then the series

$$\sum_{W\in\mathcal{W}_{0,1}}\left(\int_{p\circ p^{-1}}\omega_W\right)W.$$

As the path $p\circ p^{-1}$ is homotopically equivalent to 0, all the previous iterated integrals (for $W\neq\emptyset$) are 0. We deduce that $(\mathrm{I}_{\mathrm{KZ}})$ is equivalent to

$$\forall W\in\mathcal{W}_{0,1}\qquad \int_{p\circ p^{-1}}\omega_W=0.$$

Now, fix any $W=X_{\varepsilon_n}\cdots X_{\varepsilon_1}$ in $\mathcal{W}_{0,1}$ and compute the regularized iterated integral $\int_{p\circ p^{-1}}\omega_W$. Using (17), we have

$$\int_{p\circ p^{-1}}\omega_W=\sum_{k=0}^{n}\left(\int_p\omega_{\varepsilon_n}\circ\cdots\circ\omega_{\varepsilon_{n-k+1}}\right)\left(\int_{p^{-1}}\omega_{\varepsilon_{n-k}}\circ\cdots\circ\omega_{\varepsilon_1}\right).$$

Setting $U_1=X_{\varepsilon_n}\cdots X_{\varepsilon_{n-k+1}}$ and $U_2=X_{\varepsilon_{n-k}}\cdots X_{\varepsilon_1}$, we have

$$\int_p\omega_{\varepsilon_n}\circ\cdots\circ\omega_{\varepsilon_{n-k+1}}=(-1)^{dp(U_1)}\zeta^{ш}(U_1).$$

As p^{-1} is given by $t\mapsto 1-t$, we have for ε in $\{0,1\}$

$$(p^{-1})^*(\omega_\varepsilon)=\omega_{1-\varepsilon}.$$

Moreover, as $p^*(\omega_\varepsilon)=\omega_\varepsilon$, one computes

$$\begin{aligned}\int_{p^{-1}}\omega_{\varepsilon_{n-k}}\circ\cdots\circ\omega_{\varepsilon_1}&=\int_{0<t_1<\ldots<t_{n-k}}(p^{-1})^*(\omega_{\varepsilon_1}(t_1))\wedge\cdots\wedge(p^{-1})^*(\omega_{\varepsilon_{n-k}}(t_{n-k}))\\&=\int_{0<t_1<\ldots<t_{n-k}}\omega_{1-\varepsilon_1}(t_1)\wedge\cdots\wedge\omega_{1-\varepsilon_{n-k}}(t_{n-k})\\&=\int_p\omega_{1-\varepsilon_{n-k}}\circ\cdots\circ\omega_{1-\varepsilon_1}=\int_p\omega_{\theta(U_2)},\end{aligned}$$

where θ exchanges X_0 and X_1. Finally, we obtain

$$\int_{p^{-1}}\omega_{U_2}=\int_p\omega_{\theta(U_2)}=(-1)^{dp(\theta(U_2))}\zeta^{ш}(\theta(U_2))$$

and

$$0=\int_{p\circ p^{-1}}\omega_W=\sum_{U_1U_2=W}(-1)^{dp(U_1)}\zeta^{ш}(U_1)(-1)^{dp(\theta(U_2))}\zeta^{ш}(\theta(U_2))$$

which is exactly the relation (3) for the word W. □

Now, let c be the infinitesimal half circle around 0 in the lower half plane, connecting the tangential base point $\vec{0\infty}$ and $\vec{01}$. The path c can be seen as the limit when ε tends to 0 of $c_\varepsilon: t\mapsto\varepsilon e^{i(\pi+t\pi)}$.

We have a natural 3-cycle on $\mathcal{M}_{0,4}$ given by $\tau: t\mapsto\frac{1}{1-t}$. Let γ be the path $c\circ\tau^2(p)\circ\tau^2(c)\circ\tau(p)\circ\tau(c)\circ p$.

Theorem 3.8. *The relation* $(\mathrm{II}_{\mathrm{KZ}})$ *is equivalent to the family of relations*

$$\forall W\in\mathcal{W}_{0,1}\qquad\int_\gamma\omega_W=0$$

which is exactly the family (9)*.*

Proof. Comparing the six different normalized solutions of (KZ) at the six different base points leads to six equations. Combining these equations, one obtains $(\mathrm{II}_{\mathrm{KZ}})$ via the relation

$$g_0(u)=g_0(u)e^{i\pi X_0}\Phi_{KZ}(X_\infty,X_0)e^{i\pi X_\infty}\Phi_{KZ}(X_1,X_\infty)e^{i\pi X_1}\Phi_{KZ}(X_0,X_1)\tag{19}$$

where exponentials are coming from the relation between the solutions at the based points $0\vec{\infty}$ and $\vec{01}$ (resp. $\vec{10}$ and $1\vec{\infty}$, $\vec{\infty 1}$ and $\vec{\infty 0}$), that is, from the monodromy around 0, 1 and ∞.

Putting the six different relations together in order to get the previous equation is the same as comparing the solution g_0 with the analytic continuation of g_0 along any path starting at $\vec{01}$, joining the other tangential base points $\vec{10}$, $1\vec{\infty}$, $\vec{\infty 1}$, $\vec{\infty 0}$, $0\vec{\infty}$ in that order and ending at $\vec{01}$; staying all the time in the lower half plan. Such a path is homotopically equivalent to γ.

Thus, equation (19) gives a relation between g_0 and the solution obtained from g_0 by analytic continuation along γ. Then, the product in $U\mathfrak{F}_2$ in the R.H.S of (19) can be expressed using homotopy invariant iterated integrals as

$$e^{i\pi X_0}\Phi_{KZ}(X_\infty, X_0)e^{i\pi X_\infty}\Phi_{KZ}(X_1, X_\infty)\\ e^{i\pi X_1}\Phi_{KZ}(X_0, X_1) = \sum_{W\in\mathcal{W}_{0,1}}\left(\int_\gamma \omega_W\right)W.$$

As γ is homotopically equivalent to 0, for any word W in $\mathcal{W}_{0,1}$, one has

$$\int_\gamma \omega_W = 0.$$

This proves the first part of the theorem.

Using the decomposition of iterated integrals on a composed path (Equation (17)), we have

$$\forall W \in \mathcal{W}_{0,1} \qquad \int_\gamma \omega_W = \sum_{\substack{U_1,\dots,U_6\\ U_1\cdots U_6=W}} \int_c \omega_{U_1}\int_{\tau^2(p)}\omega_{U_2}\int_{\tau^2(c)}\omega_{U_3}\\ \int_{\tau(p)}\omega_{U_4}\int_{\tau(c)}\omega_{U_5}\int_p\omega_{U_6}.$$

Thus, in order to show that the family of relations

$$\forall W \in \mathcal{W}_{0,1} \qquad \int_\gamma \omega_W = 0$$

gives exactly the family of relations (9), it is enough to show that for any U in $\mathcal{W}_{0,1}$,

$$\int_c \omega_U = \mathrm{C}_{0,1}(e^{i\pi X_0}|U), \qquad \int_{\tau^2(p)}\omega_U = \mathrm{C}_{0,1}(\Phi_{KZ}(X_\infty, X_0)|U),$$
$$\int_{\tau^2(c)}\omega_U = \mathrm{C}_{0,1}(e^{i\pi X_\infty}|U), \qquad \int_{\tau(p)}\omega_U = \mathrm{C}_{0,1}(\Phi_{KZ}(X_1, X_\infty)|U),$$
$$\int_{\tau(c)}\omega_U = \mathrm{C}_{0,1}(e^{i\pi X_1}|U), \qquad \int_p\omega_U = \mathrm{C}_{0,1}(\Phi_{KZ}(X_0, X_1)|U).$$

In order to compute the iterated integral along c, $\tau(c)$ and $\tau^2(c)$, it is enough to compute the limit when ε tends to 0 of the iterated integral along c_ε, $\tau(c_\varepsilon)$ and $\tau^2(c_\varepsilon)$. As

$$c_\varepsilon^*(\omega_0) = i\pi\mathrm{d}t \qquad \text{and} \qquad c_\varepsilon^*(\omega_1) = \varepsilon\frac{-i\pi e^{i(\pi+\pi t)}\mathrm{d}t}{1-\varepsilon e^{i(\pi+\pi t)}},$$

the iterated integral $\int_{c_\varepsilon}\omega_U$ tends to 0 except if $U = X_0^n$ and then $\int_{c_\varepsilon}\omega_{X_0^n} = \frac{(i\pi)^n}{n!}$ for all ε. Thus, we have

$$\int_c \omega_U = \mathrm{C}_{0,1}(e^{i\pi X_0}|U).$$

Similarly we have

$$\tau(c_\varepsilon)^*(\omega_1) = i\pi\frac{\mathrm{d}t}{1-\varepsilon e^{i(\pi+\pi t)}} \qquad \text{and} \qquad \tau(c_\varepsilon)^*(\omega_0) = \frac{\varepsilon i\pi e^{i(\pi+\pi t)}\mathrm{d}t}{1-\varepsilon e^{i(\pi+\pi t)}}.$$

The iterated integral $\int_{\tau(c_\varepsilon)}\omega_U$ tends to 0 unless $U = X_1^n$, and then $\int_{c_\varepsilon}\omega_{X_0^n}$ tends to $\frac{(i\pi)^n}{n!}$ when ε tends to 0. Thus, we have

$$\int_{\tau(c)}\omega_U = \mathrm{C}_{0,1}(e^{i\pi X_1}|U).$$

Computing $\tau^2(c_\varepsilon)^*$, we have

$$\tau^2(c_\varepsilon)^*(\omega_0) = -i\pi\frac{\mathrm{d}t}{1-\varepsilon e^{i(\pi+\pi t)}} \qquad \text{and} \qquad \tau^2(c_\varepsilon)^*(\omega_1) = -i\pi\mathrm{d}t.$$

Then, we find that the limit when ε tends to 0 of $\int_{\tau^2(c_\varepsilon)}\omega_U$ is $\frac{(-i\pi)^{|U|}}{|U|!}$, which gives

$$\int_{\tau^2(c)}\omega_U = \mathrm{C}_{0,1}(e^{i\pi X_\infty}|U).$$

The equality

$$\int_p \omega_U = \mathrm{C}_{0,1}(\Phi_{KZ}(X_0,X_1)|U)$$

is obvious.

Cases of

$$\int_{\tau(p)}\omega_U \qquad \text{and} \qquad \int_{\tau^2(p)}\omega_U$$

are extremely similar and we will discuss only the last one. First, we should remark that

$$(\tau^2)^*(\omega_0) = -\omega_0+\omega_1 \qquad \text{and} \qquad (\tau^2)^*(\omega_1) = -\omega_0.$$

For $U = X_{\varepsilon_n}\cdots X_{\varepsilon_1}$ $(\varepsilon_i = 0,1)$ we can rewrite the iterated integral $\int_{\tau^2(p)}\omega_U$ as

$$\int_p (\tau^2)^*(\omega_{\varepsilon_n})\circ\cdots\circ(\tau^2)^*(\omega_{\varepsilon_1}).$$

We will now prove by induction on $n = |U|$ that in $V(\mathcal{M}_{0,4})$

$$[(\tau^2)^*(\omega_{\varepsilon_n})|\cdots|(\tau^2)^*(\omega_{\varepsilon_1})] = \sum_{(\mathbf{V},\mathbf{k})\in\mathrm{dec}_{0,1}(U,X_0)}(-1)^{|\mathbf{V}|}\omega_{X_0^{|V_1|}X_1^{k_1}X_0^{|V_2|}X_1^{k_2}\cdots X_0^{|V_p|}X_1^{k_p}} \tag{20}$$

which will give using Proposition 2.10 the equality

$$\int_{\tau^2(p)}\omega_U = \mathrm{C}_{0,1}(\Phi_{KZ}(X_0,X_1)|U).$$

If $U = X_0$, the set $\mathrm{dec}_{0,1}(U,X_0)$ has 2 elements $((X_0),(0))$ and $((\emptyset),(1))$. Similarly, if $U = X_1$ then $\mathrm{dec}_{0,1}(U,X_0)$ has only one element which is $((X_1),(0))$. In both cases (20) is satisfied.

Let $U = X_{\varepsilon_n}\cdots X_{\varepsilon_1}$ be a word in $\mathcal{W}_{0,1}$, and let ε be in $\{0,1\}$. For the simplicity of notation, we shall write $[\omega_{\varepsilon_n}|\cdots|\omega_{\varepsilon_1}|\omega_\varepsilon]$ as

$$[\omega_U|\omega_\varepsilon] := [\omega_{\varepsilon_n}|\cdots|\omega_{\varepsilon_1}|\omega_\varepsilon].$$

We suppose now that

$$U = U_1X_0 \qquad\qquad \text{with } |U_1| \geqslant 1.$$

We have a map from $\mathrm{dec}_{0,1}(U,X_0)$ to $\mathrm{dec}_{0,1}(U_1,X_0)$ that sends a decomposition

$$(\mathbf{V},\mathbf{k}) = ((V_1,\ldots,V_p),(k_1,\ldots,k_p))$$

to

$$\begin{cases} (\mathbf{V}, (k_1, \ldots, k_p - 1)) & \text{if } k_p \neq 0 \\ ((V_1, \ldots, V_p'), \mathbf{k}) & \text{if } k_p = 0 \text{ and } V_p = V_p' X_0. \end{cases}$$

Any decomposition $(\mathbf{V}', \mathbf{k}')$ in $\operatorname{dec}_{0,1}(U_1, X_0)$ has exactly two preimages by this map. If one writes

$$U_1 = V_1' X_0^{k_1'} \cdots V_1' X_0^{k_p'}$$

then it leads to two decompositions of U

$$((V_1', \ldots, V_p'), (k_1', \ldots, k_p' + 1)) \qquad \text{and} \qquad ((V_1', \ldots, V_p', X_0), (k_1', \ldots, k_p', 0)).$$

By induction we have in $V_{n-1}(\mathcal{M}_{0,4})$

$$[(\tau^2)^*(\omega_{\varepsilon_n})| \cdots |(\tau^2)^*(\omega_{\varepsilon_2})] = \sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} \omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'}}.$$

We deduce from the previous equality and using the linearity of the tensor product that $[(\tau^2)^*(\omega_{\varepsilon_n})| \cdots |(\tau^2)^*(\omega_{\varepsilon_1})]$ is equal to

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} [\omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'}} | -\omega_0 + \omega_1].$$

This sum can be decomposed as

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|+1} [\omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'}} |\omega_0] +$$

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} [\omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'}} |\omega_1].$$

The first term of the sum is equal to

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|+1} \omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'} X_0}$$

and the second term is equal to

$$\sum_{\substack{(\mathbf{V}', \mathbf{k}') \in \\ \operatorname{dec}_{0,1}(U_1, X_0)}} (-1)^{|\mathbf{V}'|} \omega_{X_0^{|V_1'|} X_1^{k_1'} \cdots X_0^{|V_p'|} X_1^{k_p'+1}}.$$

The previous discussion on $\operatorname{dec}_{0,1}(U, X_0)$ tells us that adding the two sums above gives

$$\sum_{(\mathbf{V}, \mathbf{k}) \in \operatorname{dec}_{0,1}(U, X_0)} (-1)^{|\mathbf{V}|} \omega_{X_0^{|V_1|} X_1^{k_1} X_0^{|V_2|} X_1^{k_2} \cdots X_0^{|V_p|} X_1^{k_p}}.$$

This gives (20) when $U = U_1 X_0$.

If $U = U_1 X_1$ with $|U_1| \geqslant 1$, we have a one to one correspondence between $\operatorname{dec}_{0,1}(U_1, X_0)$ and $\operatorname{dec}_{0,1}(U, X_0)$ defined by

$$((V_1', \ldots, V_p'), (k_1', \ldots, k_p')) \mapsto \begin{cases} ((V_1', \ldots, V_p', X_1), (k_1', \ldots, k_p', 0)) & \text{if } k_p' > 0 \\ ((V_1', \ldots, V_p' X_1), (k_1', \ldots, k_p')) & \text{otherwise.} \end{cases}$$

Then (20) follows by induction using the linearity of the tensor product. $\square$

3.3. **Bar Construction on $\mathcal{M}_{0,5}$ and the pentagon relations.** Here, we will show how the pentagon relations ($\mathrm{III}_{\mathrm{KZ}}$) are related to the bar construction on $\mathcal{M}_{0,5}$.

The shuffle algebra $B(\mathcal{M}_{0,5})$ being much more complicated than $B(\mathcal{M}_{0,4})$ we will first review some facts explained in [Bro09]. We now fix a dihedral structure δ, as described in [Bro09], on $\mathcal{M}_{0,5}$. We will used the "standard" dihedral structure given by "cyclic" order on the marked points

$$z_1 < z_2 < z_3 < z_4 < z_5 (< z_1)$$

or with our normalization

$$0 < xy < y < 1 < \infty.$$

This corresponds to a good choice of coordinates to study the connected components of $\mathcal{M}_{0,5}(\mathbb{R})$ such that the marked points are in the order given by δ. We will refer to that component as the standard cell.

More precisely, let i, j, k, l denote distinct elements of $\{1, 2, 3, 4, 5\}$. The cross-ratio $[i\, j|k\, l]$ is defined by the formula:

$$[i\, j|k\, l] = \frac{z_i - z_k}{z_i - z_l} \frac{z_j - z_l}{z_j - z_k}.$$

Brown, in [Bro09, Sections 2.1 and 2.2], has defined coordinates on $\mathcal{M}_{0,n}$, and more generally on an open $\mathcal{M}^{\delta}_{0,n}$ of the Deligne-Mumford compactification of the moduli space of curves $\overline{\mathcal{M}_{0,n}}$, such that

$$\mathcal{M}_{0,n} \subset \mathcal{M}^{\delta}_{0,n} \subset \overline{\mathcal{M}_{0,n}}.$$

These coordinates respect the natural dihedral symmetry of the moduli spaces of curves. Applying his work to the case $n = 5$, let i and j be in $\{1, 2, 3, 4, 5\}$ such that i, $i + 1$, j and $j + 1$ are distinct. We set

$$u_{ij} = [i\, i + 1|j + 1\, j].$$

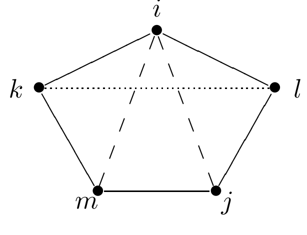
In particular, the codimension 1 components of $\partial\mathcal{M}_{0,n}$ contained in $\mathcal{M}^{\delta}_{0,n}$ are given by $u_{ij} = 0$ and the standard cell is contained in $\mathcal{M}^{\delta}_{0,n}$.

The coordinates u_{ij} satisfy the relations

$$u_{ij}u_{im} + u_{kl} = 1, \tag{21}$$

for $k \equiv i - 1 \mod 5$, $l \equiv i + 1 \mod 5$ and $m \equiv j + 1 \mod 5$, all the indices being in $\{1, 2, 3, 4, 5\}$ and such that u_{ij}, u_{im} and u_{kl} are defined.

In [Bro09][Corollary 2.3], these relations are given in terms of two sets of chords of a polygon (a pentagon for $\mathcal{M}_{0,5}$) and the picture corresponding to the above relation is given below.



Let ω_{12}, ω_{23}, ω_{34}, ω_{45}, ω_{24} be the differential forms

$$\omega_{12} = \mathrm{d}\log(u_{25}) = \frac{\mathrm{d}x}{x}, \quad \omega_{23} = \mathrm{d}\log(u_{31}u_{41}) = \frac{\mathrm{d}x}{x-1},$$
$$\omega_{34} = \mathrm{d}\log(u_{24}u_{41}) = \frac{\mathrm{d}y}{y-1}, \quad \omega_{45} = \mathrm{d}\log(u_{35}) = \frac{\mathrm{d}y}{y}$$
$$\text{and} \quad \omega_{24} = \mathrm{d}\log(u_{41}) = \frac{\mathrm{d}(xy)}{xy-1}.$$

If W is a word in $\mathcal{W} = \{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*$ with $|W| = n$, we will write $\omega_W \in \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M}_{0,5})^{\otimes n}$ for the bar symbol $[\omega_{i_n j_n}|\cdots|\omega_{i_1 j_1}]$. Note that the elements ω_W for W in $\mathcal{W}$ are not all in $V(\mathcal{M}_{0,5})$; in general, only linear combinations of such symbols are in $V(\mathcal{M}_{0,5})$.

Example 3.9. The elements $[\omega_{12}]$, $[\omega_{23}]$ and $[\omega_{12}|\omega_{23}]$ are in $V(\mathcal{M}_{0,5})$ even if $[\omega_{12}|\omega_{45}]$ is not. However $[\omega_{12}|\omega_{45}] + [\omega_{45}|\omega_{12}]$ is in $V(\mathcal{M}_{0,5})$.

Example 3.43 in [Bro09] (using [Bro09, Thm. 3.38 and Coro. 3.41]) tells us that the exact sequence

$$0 \longrightarrow \mathbb{C}\langle\langle X_{24}, X_{34}, X_{45}\rangle\rangle \longrightarrow U\mathfrak{B}_5 \longrightarrow \mathbb{C}\langle\langle X_{12}, X_{23}\rangle\rangle \longrightarrow 0$$

is dual to the exact sequence

$$0 \longrightarrow V(\mathcal{M}_{0,4}) \longrightarrow V(\mathcal{M}_{0,5}) \longrightarrow \mathbb{C}\langle\frac{\mathrm{d}y}{y}, \frac{\mathrm{d}y}{y-1}, \frac{x\,\mathrm{d}y}{xy-1}\rangle \longrightarrow 0$$

which comes from the expression, in cubical coordinates, of the map $\mathcal{M}_{0,5} \longrightarrow \mathcal{M}_{0,4}$ which forgets the 4^{Th} point. Thus, the identification

$$U\mathfrak{B}_5 \simeq \mathbb{C}\langle\langle X_{24}, X_{34}, X_{45}\rangle\rangle \rtimes \mathbb{C}\langle\langle X_{12}, X_{23}\rangle\rangle$$

is dual (as graded algebra) to

$$V(\mathcal{M}_{0,5}) \simeq V(\mathcal{M}_{0,4}) \otimes \mathbb{C}\langle\frac{\mathrm{d}y}{y}, \frac{\mathrm{d}y}{y-1}, \frac{x\,\mathrm{d}y}{xy-1}\rangle$$

and $V(\mathcal{M}_{0,5})$ is the graded dual $U\mathfrak{B}_5^*$ of $U\mathfrak{B}_5$.

The graded dual of the free non-commutative algebra of formal series

$$R = \mathbb{C}\langle\langle X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\rangle\rangle$$

is the shuffle algebra

$$T := \bigoplus_n (\mathbb{C}\omega_{34} \oplus \mathbb{C}\omega_{45} \oplus \mathbb{C}\omega_{24} \oplus \mathbb{C}\omega_{12} \oplus \mathbb{C}\omega_{23})^{\otimes n}.$$

Let Ω be the element in $R \otimes \mathrm{H}^1_{\mathrm{DR}}(\mathcal{M}_{0,5})$ defined by

$$\Omega = X_{12} \otimes \omega_{12} + X_{23} \otimes \omega_{23} + X_{34} \otimes \omega_{34} + X_{45} \otimes \omega_{45} + X_{24} \otimes \omega_{24}.$$

and

$$\mathrm{Exp}(\Omega) := \sum_{W \in \mathcal{W}} W \otimes \omega_W \in R \otimes T.$$

The element $\mathrm{Exp}(\Omega)$ corresponds to the identity of R and encodes the fact that the dual of a word W is ω_W. A word W (seen in $U\mathfrak{B}_5$) is written in the basis B_4 as

$$W = \sum_{b_4 \in B_4} l_{b_4,W} b_4.$$

Duality between R and T and between $U\mathfrak{B}_5$ and $V(\mathcal{M}_{0,5})$ tells us that, the basis $B_4^* = (b_4^*)_{b_4 \in B_4}$ of $V(\mathcal{M}_{0,5})$ dual to B_4 is given by

$$\forall b_4 \in B_4 \qquad b_4^* = \sum_{W \in \mathcal{W}} l_{b_4,W}\,\omega_W.$$

Using the projection $R \to U\mathfrak{B}_5$ one can see $\mathrm{Exp}(\Omega)$ in $U\mathfrak{B}_5 \otimes T$. Actually, by duality, $\mathrm{Exp}(\Omega)$ lies in $U\mathfrak{B}_5 \otimes V(\mathcal{M}_{0,5})$. So, writing each W in the basis B_4 leads to the following expression of $\mathrm{Exp}(\Omega)$ in $U\mathfrak{B}_5 \otimes V(\mathcal{M}_{0,5})$

$$\mathrm{Exp}(\Omega) = \sum_{b_4 \in B_4} b_4 \otimes b_4^* \quad \in U\mathfrak{B}_5 \otimes V(\mathcal{M}_{0,5}).$$

Thus, $\mathrm{Exp}(\Omega)$ realized the identification between the graded dual of $U\mathfrak{B}_5$ and $V(\mathcal{M}_{0,5})$ as was observed by Furusho in [Fur08]. This discussion can be summarized by the following proposition.

Proposition 3.10. *We have a natural identification*

$$U\mathfrak{B}_5^* \simeq V(\mathcal{M}_{0,5}),$$

$U\mathfrak{B}_5^*$ *being the graded dual of* $U\mathfrak{B}_5$.

This identification gives a basis B_4^* *of* $V(\mathcal{M}_{0,5})$ *dual to* B_4 *the basis of* $U\mathfrak{B}_5$ *which comes from the identification*

$$U\mathfrak{B}_5 \simeq \mathbb{C}\langle\langle X_{24}, X_{34}, X_{45}\rangle\rangle \rtimes \mathbb{C}\langle\langle X_{12}, X_{23}\rangle\rangle.$$

The basis $B_4^* = (b_4^*)_{b_4 \in B_4}$ *is explicitly given for all* b_4 *in the basis* B_4 *by*

$$b_4^* = \sum_{W \in \mathcal{W}} l_{b_4,W}\, \omega_W. \tag{22}$$

Let $\widehat{\mathcal{M}_{0,5}}$ be the universal covering of $\mathcal{M}_{0,5}$. A multi-valued function on $\mathcal{M}_{0,5}$ is an analytic function on $\widehat{\mathcal{M}_{0,5}}$. Consider the formal differential equation on $\widehat{\mathcal{M}_{0;5}}$

$$\mathrm{d}L = \Omega L$$

where L takes values in $U\mathfrak{B}_5$, whose coefficients are multi-valued functions on $\mathcal{M}_{0,5}$. As in the case of the equation (KZ), if we fix either the value of L at some point of $\mathcal{M}_{0,5}$ or its asymptotic behavior at a tangential base point, then the solution is unique.

The irreducible components of codimension 1 of $\partial\mathcal{M}_{0,5}$ in $\overline{\mathcal{M}_{0,5}}$ are in one to one correspondence with the 2-partitions of $\{z_1, z_2, z_3, z_4, z_5\}$ and will be denoted as $z_{i_1} z_{i_2} | z_{i_3} z_{i_4} z_{i_5}$. These boundary components are all isomorphic to $\overline{\mathcal{M}_{0,4}}$. Here, we will only consider the following components $\bar{D}_{52} = z_1 z_2 | z_3 z_4 z_5$, $\bar{D}_{13} = z_2 z_3 | z_4 z_5 z_1$, $\bar{D}_{24} = z_3 z_4 | z_5 z_1 z_2$, $\bar{D}_{35} = z_4 z_5 | z_1 z_2 z_3$, $\bar{D}_{41} = z_5 z_1 | z_2 z_3 z_4$ (we may use the convention $\bar{D}_{ij} = \bar{D}_{ji}$). One remarks that those components are given by a partition that respect the dihedral structure δ and the numbering $\bar{D}_{ij}$ is coherent with the notation of [Bro09]. We will write $D_{ij} \simeq \mathcal{M}_{0,4}^{\delta}$ for the intersection of $\bar{D}_{ij}$ with $\mathcal{M}_{0,5}^{\delta}$. The divisors D_{ij} are given in the dihedral coordinates by $u_{ij} = 0$. Following Brown, we have 5 tangential base points (corresponding to the intersection of 2 irreducible components) given by the triangulation of the polygon corresponding to δ; as we are working in $\mathcal{M}_{0,5}$, the polygon is a pentagon, and a triangulation is given by two chords going out from a single vertex, so one can number the triangulation by the number of its vertex: precisely, one has

$$\begin{aligned} &P_3 = D_{35} \cap D_{13}, \qquad P_1 = D_{13} \cap D_{41}, \qquad P_4 = D_{41} \cap D_{24}, \\ &P_2 = D_{24} \cap D_{52}, \qquad \text{and} \qquad P_5 = D_{52} \cap D_{35}. \end{aligned}$$

Let L_i be the normalized solution at P_i (see [Bro09] Theorem 6.12).

Now, we fix a basis $B = (b)_{b \in B}$ of $U\mathfrak{B}_5$ and its dual basis $B^* = (b^*)_{b \in B}$ in $V(\mathcal{M}_{0,5})$. The description of the situation in dimension 1 and section 5.2 in [Bro09] shows that Theorem 6.27 of Brown's article in [Bro09] can be rewritten as follows.

Proposition 3.11. *For any tangential base point P_i, one can write $L_i(z)$ as*

$$\forall z \in \widehat{\mathcal{M}_{0,5}} \quad L_i(z) = \sum_{b \in B} (\int_\gamma b^*) b$$

where γ is a path from P_i to z and where iterated integrals are regularized iterated integrals.

The comparison of two different normalized solutions at two different base points P_i and P_j is then given by

$$\forall z \in \widehat{\mathcal{M}_{0,5}} \qquad L_i(z) = L_j(z) \left(\sum_{b \in B} \left(\int_\gamma b^* \right) b \right)$$

where γ is any path going from P_i to P_j homotopically equivalent to a path γ' going from P_i to P_j in the standard cell of $\mathcal{M}_{0,5}(\mathbb{R})$.

Brown shows how to restrict any element ω in $B(\mathcal{M}_{0,5})$ to any boundary components D introducing a regularization map $\mathrm{Reg}(\omega, D)$. This map sends each $\frac{\mathrm{d}u_{ij}}{u_{ij}}$ to 0 if the restriction of u_{ij} to D equals 0 or 1. More precisely,

Definition 3.12. Let D_{ij} be a boundary component of $\mathcal{M}_{0,n}$ given by $u_{ij} = 0$. We define $\mathrm{Reg}(\frac{\mathrm{d}u_{kl}}{u_{kl}}, D_{ij})$ as follows:

- $\mathrm{Reg}(\frac{\mathrm{d}u_{ij}}{u_{ij}}, D_{ij}) = 0$,
- $\mathrm{Reg}(\frac{\mathrm{d}u_{kl}}{u_{kl}}, D_{ij}) = 0$ if $u_{ij}u_{im} + u_{kl} = 1$ as in (21),
- $\mathrm{Reg}(\frac{\mathrm{d}u_{kl}}{u_{kl}}, D_{ij}) = \frac{\mathrm{d}\tilde{u_{kl}}}{\tilde{u_{kl}}}$ where $\tilde{u_{kl}}$ is the restriction of u_{kl} to D_{ij} using the natural inclusion
$$D_{ij} \hookrightarrow \mathcal{M}^\delta_{0,5}.$$

Now, using the inclusion $\mathcal{M}_{0,4} \hookrightarrow \mathcal{M}^\delta_{0,4} \simeq D_{ij}$, one can define the map

$$\mathrm{Reg}(-, D_{ij}) : V(\mathcal{M}_{0,5}) \longrightarrow V(\mathcal{M}_{0,4}).$$

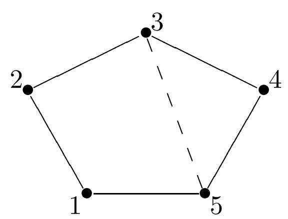
It sends an element

$$\omega = \sum c_{i_1,j_1,\dots,i_k,j_k} [\omega_{i_1 j_1} | \dots | \omega_{i_k j_k}] \in V(\mathcal{M}_{0,5})$$

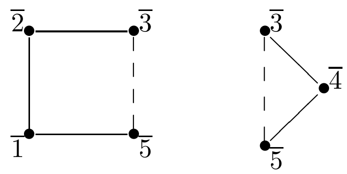
to

$$\mathrm{Reg}(\omega, D_{ij}) = \sum c_{i_1,j_1,\dots,i_k,j_k} [\mathrm{Reg}(\omega_{i_1 j_1}, D_{ij}) | \dots | \mathrm{Reg}(\omega_{i_k j_k}, D_{ij})] \in V(\mathcal{M}_{0,4}).$$

Example 3.13. As explained in Brown [Bro09, Lemma 2.6], the restriction of the coordinate u_{25} on D_{35} can be computed in terms of the dihedral coordinates on $D_{35} \simeq \mathcal{M}^\delta_{0,4}$ as follows. The chord $(3,5)$ splits the pentagon



into a square and a triangle



,

where we have written $\bar{i}$ instead of i to keep track of the difference between the labeling on the pentagon (corresponding to $\mathcal{M}_{0,5}^{\delta}$) and the square (corresponding to $\mathcal{M}_{0,4}^{\delta} \simeq D_{35}$).

This decomposition corresponds to the isomorphism

$$D_{35} \xrightarrow{\sim} \mathcal{M}_{0,4}^{\delta} \times \mathcal{M}_{0,3}^{\delta} \xrightarrow{\sim} \mathcal{M}_{0,4}^{\delta}$$

where, in $\mathcal{M}_{0,4} \subset \mathcal{M}_{0,4}^{\delta}$, the four marked points are labeled $z_{\overline{1}}$, $z_{\overline{2}}$, $z_{\overline{3}}$ and $z_{\overline{5}}$.

The coordinate u_{25} is given by the cross-ratio

$$u_{25} = [23|15].$$

Its restriction to D_{35} is the coordinate given by the chord $(\overline{2}, \overline{5})$ and thus by the cross-ratio

$$\tilde{u_{25}} = [\overline{23}|\overline{15}].$$

Following this description, there are two dihedral coordinates on $D_{35} \simeq \mathcal{M}_{0,4}^{\delta}$ given by

$$t_1 = [\overline{23}|\overline{15}] \qquad \text{and} \qquad t_2 = [\overline{12}|\overline{35}].$$

Similarly, u_{13}, corresponding to the chords $(1,3)$ in the pentagon description, restricts on D_{35} to t_2 which corresponds to the chord $(\overline{1}, \overline{3})$ on the square description of D_{35}. As P_5 is defined by $u_{25} = u_{35} = 0$, one sees that $t_1 = \tilde{u_{25}}$ is 0 at P_5 and similarly that $t_2 = \tilde{u_{13}}$ is 0 at P_3. Moreover, on D_{35} one has $t_2 = 1 - t_1$, which agrees with the fact that on $\mathcal{M}_{0,5}$ one has $u_{25} + u_{13}u_{14} = 1$ and $u_{14} + u_{25}u_{35} = 1$. Thus, the coordinate t_1 is equal to 1 at P_3 and t_2 is equal to 1 at P_5.

Proposition 3.14. *For any two consecutive tangential base points P_i and P_j with $j \equiv i - 2 \mod 5$, one has*

$$\forall z \in \widehat{\mathcal{M}_{0,5}} \qquad L_i(z) = L_j(z) \left(\sum_{b \in B} \left(\int_{p_{ji}} \mathrm{Reg}(b^*, D_{ji}) \right) b \right)$$

where p_{ji} is the real segment going in D_{ji} from P_i to P_j.

Proof. The symmetry of the situation allows us to prove it only in the case where $i = 5$, $j = 3$ and B is the basis B_4.

Let p_{35} be the path in D_{35} going from P_5 to P_3; we need to show that

$$L_3(z)^{-1} L_5(z) = \sum_{b_4 \in B_4} \left(\int_{p_{35}} \mathrm{Reg}(b_4^*, D_{35}) \right) b_4. \tag{23}$$

Brown, in [Bro09, Definition 6.18], defined Z^{35} to be the quotient $L_3(z)^{-1}L_5(z)$. Using the proof of Theorem 6.20 in [Bro09], we have

$$Z^{35} = L_3(z)^{-1} L_5(z) = \sum_{\substack{W = X_{i_n j_n} \cdots X_{i_1 j_1} \\ \in \{X_{12}, X_{23}\}^*}} \left(\int_p \frac{\mathrm{d}t}{t - \varepsilon_n} \wedge \cdots \wedge \frac{\mathrm{d}t}{t - \varepsilon_1} \right) W$$

with $\varepsilon_k = 0$ if $i_k = 1$ (and $j_k = 2$)) and $\varepsilon_k = 1$ otherwise (that is, $i_k = 2$ and $j_k = 3$). Using the morphism $p_4 : U\mathfrak{B}_5 \longrightarrow U\mathfrak{F}_2$ that send X_{i4} to 0, X_{12} to X_0 and X_{23} to X_1, we have:

$$Z^{35} = L_3(z)^{-1} L_5(z) = \sum_{\substack{W = X_{i_n j_n} \cdots X_{i_1 j_1} \\ \in \{X_{12}, X_{23}\}^*}} \left(\int_p \omega_{p_4(W)} \right) W.$$

We recall that an element b_4 of the basis B_4 is either 1 or a monomial of the form

$$b_4 = U_{245} V_{123} \qquad U_{245} \in \{X_{24}, X_{34}, X_{45}\}^*, \quad V_{123} \in \{X_{12}, X_{23}\}^*. \tag{24}$$

So, in order to prove (23), it is enough to prove that:

- All the iterated integrals $\int_{p_{35}} \mathrm{Reg}(b_4^*, D_{35})$ for $b_4 = U_{245}V_{123}$ with U_{245} not empty vanish:

$$\left.\begin{array}{c} b_4 = U_{245}V_{123} \\ \text{with } U_{245} \in \{X_{24}, X_{34}, X_{45}\}^*, \quad U_{245} \neq \emptyset \end{array}\right\} \quad \Rightarrow \quad \int_{p_{35}} \mathrm{Reg}(b_4^*, D_{35}) = 0.$$

- All the iterated integrals $\int_{p_{35}} \mathrm{Reg}(b_4^*, D_{35})$ for $b_4 = V_{123}$ are equal to

$$\int_p \omega_{p_4(V_{123})} = \int_p \omega_{p_4(b_4)}.$$

  That is:

$$b_4 = V_{123} \in \{X_{12}, X_{23}\}^* \quad \Rightarrow \quad \int_{p_{35}} \mathrm{Reg}(b_4^*, D_{35}) = \int_p \omega_{p_4(b_4)}.$$

Let t denote the dihedral coordinate t_1 on D_{35} which takes values 0 at P_5 and 1 at P_3 (see Example 3.13). Example 3.13 shows that

$$\tilde{u_{25}} = t, \qquad \tilde{u_{13}} = 1 - t.$$

Moreover, as

$$u_{24} + u_{13}u_{35} = 1 \qquad \text{and} \qquad u_{14} + u_{25}u_{35} = 1,$$

one has $u_{24} = u_{14} = 1$ on D_{35}.

As the differential forms ω_{23} and ω_{34} are defined by

$$\begin{aligned} \omega_{23} &= \mathrm{d}\log(u_{31}u_{41}) = \mathrm{d}\log(u_{13}) + \mathrm{d}\log(u_{14}) \qquad \text{and} \\ \omega_{34} &= \mathrm{d}\log(u_{24}u_{41}) = \mathrm{d}\log(u_{24}) + \mathrm{d}\log(u_{14}), \end{aligned}$$

and since one has

$$\mathrm{Reg}(\mathrm{d}\log(u_{35}), D_{35}) = \mathrm{Reg}(\mathrm{d}\log(u_{24}), D_{35}) = \mathrm{Reg}(\mathrm{d}\log(u_{14}), D_{35}) = 0,$$

one concludes that

$$\begin{aligned} \mathrm{Reg}(\omega_{12}, D_{35}) &= \mathrm{Reg}(\mathrm{d}\log(u_{25}), D_{35}) = \frac{\mathrm{d}t}{t}, \\ \mathrm{Reg}(\omega_{23}, D_{35}) &= \mathrm{Reg}(\mathrm{d}\log(u_{13}), D_{35}) = \frac{\mathrm{d}t}{t-1} \end{aligned}$$

and $\mathrm{Reg}(\omega_{ij}, D_{35}) = 0$ otherwise.

It is now enough to show that for b_4 in B_4

- b_4 is a word in the letters X_{12} and X_{23} (that is $b_4 \in \{X_{12}, X_{23}\}^*$) if and only if

$$\begin{aligned} & b_4^* = \omega_{b_4} \quad \text{with } b_4 \in \{X_{12}, X_{23}\}^* \\ & (= [\omega_{i_n j_n} | \cdots | \omega_{i_1 j_1}] \quad \text{with } X_{i_k j_k} \in \{X_{12}, X_{23}\}) \end{aligned}$$

- b_4 contains some X_{ij} with $i = 4$ or $j = 4$ if and only if

$$b_4^* = \sum \lambda_{W'} \omega_{W'} \quad \text{with} \quad \lambda_{W'} \neq 0 \Rightarrow W' \notin \{X_{12}, X_{23}\}^*$$

  that is, if and only if b_4^* is a linear combination of bar symbols $\sum \lambda_{W'}\omega_{W'}$ ($\lambda_{W'} \neq 0$) with W' containing at least one of the letters X_{34}, X_{45}, X_{24}.

Using equations (24) and (22) that describe respectively b_4 and b_4^*, one sees that Equation (23) (and thus the proposition) follows directly from the relation defining $U\mathfrak{B}_5$. □

From the previous proposition, we immediately deduce the following corollary.

Corollary 3.15. *For any path γ in the standard cell homotopically equivalent to p_{ji} $j \equiv i - 2 \mod 5$ ($1 \leqslant i, j \leqslant 5$), we have*

$$\forall \omega \in V(\mathcal{M}_{0,5}) \qquad \int_\gamma \omega = \int_{p_{ji}} \mathrm{Reg}(\omega, D_{ji}).$$

Let $\gamma = p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$ denote the composed path beginning and ending at P_3 and extending the map $\mathrm{Reg}(\omega, \gamma)$ to paths that are piecewise in some of the divisor D_{ij}.

Theorem 3.16. *The relation* ($\mathrm{III}_{\mathrm{KZ}}$) *is equivalent to the family of relations*

$$\forall b_4 \in B_4,\ b_4 \neq 1 \qquad \int_\gamma \mathrm{Reg}(b_4^*, \gamma) = 0$$

which is exactly the family (14).

Proof. For i in $\{1,2,3,4,5\}$ and $j = i-2 \mod 5$, we define Z^{ji} by the formula

$$Z^{ji} = \left(\sum_{b_4 \in B_4} \left(\int_{p_{ji}} \mathrm{Reg}(b_4^*, D_{ji}) \right) b_4 \right).$$

By Proposition 3.14, one has

$$\forall z \in \widehat{\mathcal{M}_{0,5}} \qquad L_i(z) = L_j(z) Z^{ji}.$$

Comparison between the 5 normalized solutions L_i at the 5 tangential base points P_i gives

$$\forall z \in \widehat{\mathcal{M}_{0,5}} \qquad L_3(z) = L_3(z) Z^{35} Z^{52} Z^{24} Z^{41} Z^{13}. \tag{25}$$

In the proof of Theorem 6.20 [Bro09] and the example which follows it, Brown proves that the product of the Z^{ji} is equal to the L.H.S (that is the product of the Φ_{KZ}) of ($\mathrm{III}_{\mathrm{KZ}}$). So, Equation ($\mathrm{III}_{\mathrm{KZ}}$) can be written as

$$Z^{35} Z^{52} Z^{24} Z^{41} Z^{13} = 1.$$

It can also be proved directly using Proposition 3.14.

Equation (25) is given by the analytic continuation of the solution L_3 along any path in the standard cell beginning and ending at P_3 and going through P_1, P_4, P_2 and P_5 (in that order). Such a path is homotopically equivalent to γ (and to 0) and the product of the Z^{ji} can be written as

$$Z^{35} Z^{52} Z^{24} Z^{41} Z^{13} = \sum_{b_4 \in B_4} \left(\int_\gamma b_4^* \right) b_4.$$

As γ is homotopically equivalent to 0, each of the homotopy invariant regularized iterated integrals above are 0 (except for $b_4 = 1$). Thus, the product

$$Z^{35} Z^{52} Z^{24} Z^{41} Z^{13}$$

is equal to 1. We deduce from the previous discussion that the family of relations

$$\forall b_4 \in B_4,\ b_4 \neq 1 \qquad \int_\gamma \mathrm{Reg}(b_4^*, \gamma) = 0$$

implies relation ($\mathrm{III}_{\mathrm{KZ}}$). Moreover, one deduces from the equation

$$Z^{35} Z^{52} Z^{24} Z^{41} Z^{13} = \sum_{b_4 \in B_4} \left(\int_\gamma b_4^* \right) b_4.$$

that relation ($\mathrm{III}_{\mathrm{KZ}}$) (which says that the product of the Z^{ji} is 1) implies

$$\forall b_4 \in B_4,\ b_4 \neq 1 \qquad \int_\gamma \mathrm{Reg}(b_4^*, \gamma) = 0.$$

The first part of the theorem is then proved.

Using the expression of b_4^* in terms of ω_W, the end of the theorem follows from Proposition 3.18 below. □

From the previous theorem, one deduces the following corollary.

Corollary 3.17. *For any basis B of $U\mathfrak{B}_5$, the pentagon relation* (III$_{\mathrm{KZ}}$) *is equivalent to*

$$\forall b \in B \qquad \int_\gamma \mathrm{Reg}(b^*, \gamma) = 0$$

where γ, as previously, is the path $p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$.

Following the proof of 3.14, one proves Proposition 3.18, which completes the proof of Theorem 3.16.

Proposition 3.18. *For any bar symbol ω_W dual to a word W in the letters X_{34}, X_{45}, X_{24}, X_{12}, X_{23}, we have*

$$C_{5,W,KZ} = \int_\gamma \mathrm{Reg}(\omega_W, \gamma)$$

where $C_{5,W,KZ}$ is the coefficient $C_{5,W}$ defined in (10) *in the particular case of the Drinfel'd associator Φ_{KZ}.*

Proof. To show the proposition, it is enough, using the decomposition of $\gamma = p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$, to show that for any U in $\{X_{34}, X_{45}, X_{24}, X_{12}, X_{23}\}^*$ and any i, one has

$$(-1)^{dp_i(U)} \zeta^{ш}(\rho_i(U)) = \int_{I_i} \mathrm{Reg}(\omega_U, I_i)$$

where $I_5 = p_{13}$, $I_4 = p_{41}$, $I_3 = p_{24}$, $I_2 = p_{52}$ and $I_1 = p_{35}$.

As $\mathrm{Reg}(\omega_{kl}, I_i) = \omega_{\rho_i(X_{kl})}$, the proposition follows. □

4. Appendix : relations in low degrees

4.1. **Remarks.** From the following tables, one can see that coefficients of words in X_{12} and X_{23} yield the family of relations (2) (which is equivalent to (I)). This can be proved directly from (13) (which is equivalent to (III)). In order to do so, one observes that if b_4 in the basis B_4 is a word in X_{12} and X_{23}, then $l_{b_4,W} \neq 0$ if and only if $W = b_4$. In the case of the Drinfel'd associator Φ_{KZ}, only the term

$$\sum_{U_1 \cdots U_5 = b_4} (-1)^{dp_1(U_1)+dp_2(U_2)+dp_3(U_3)+dp_4(U_4)+dp_5(U_5)}$$
$$\zeta^{ш}(\rho_1(U_1))\zeta^{ш}(\rho_2(U_2))\zeta^{ш}(\rho_3(U_3)\zeta^{ш}(\rho_4(U_4))\zeta^{ш}(\rho_5(U_5))$$

is non zero, and the U_i are words in X_{12} and X_{23}. Then, the fact that $\rho_2(X_{12}) = \rho_2(X_{23}) = 0$ tells us that $\rho_2(U_2) = 0$ if $U_2 \neq \emptyset$. As $\rho_4(X_{12}) = \rho_5(X_{12}) = 0$, $\rho_4(X_{23}) = X_0$ and $\rho_5(X_{23}) = X_1$, we deduce that $\rho_4(U_4)$ is 0 or a power of X_0 and $\rho_5(U_5)$ is 0 or a power of X_1 (again with $U_4, U_5 \neq \emptyset$). We conclude using the fact that for $k \geqslant 1$,

$$\zeta^{ш}(0) = \zeta^{ш}(X_0^k) = \zeta^{ш}(X_1^k) = 0.$$

Using the explicit relations between the coefficients of the associator (13), the above arguments show the well known implication "(III) implies (I)" proved by Furusho in [Fur03].

In [Fur10], Furusho also proved that (III) implies (II). This implication does not appear clearly looking at the coefficients and comparing (13) and (8). In the case of Φ_{KZ}, the first reason is that no π can arise from (14). In order to see "(III) implies (II)" on the coefficients, one should first replace $(2\pi i)^2$ by $-24\zeta^{ш}(X_0X_1)$ in (9). The second reason is that the proof of Furusho suggests that the linear combinations involved are much more complicated than the ones involved for (III) implies (I) (which is deduced from (III) by sending $X_{i,4}$ to 0).

Another set of well-known relations between multiple zeta values are the double shuffle relations. As the representation of the multiple zeta values with iterated integrals leads to the quadratic relations

$$\zeta^{ш}(V)\zeta^{ш}(W) = \sum_{U\in \mathrm{sh}(V,W)} \zeta^{ш}(U),$$

writing the multiple zeta values as series $\zeta(\mathbf{k}) = \sum \frac{1}{n_1^{k_1}\cdots n_p^{k_p}}$ leads to another regularization ζ^* and another set of quadratic relations ([Rac02])

$$\zeta^*(\mathbf{k})\zeta^*(\mathbf{l}) = \sum_{\mathbf{m}\in \mathrm{st}(\mathbf{k},\mathbf{l})} \zeta^*(\mathbf{m})$$

where $\mathrm{st}(\mathbf{k},\mathbf{l})$ is a family of tuples of integers defined from $\mathbf{k}$ and $\mathbf{l}$ by a combinatorial process. The two regularizations are linked by an explicit formula, and the set of relations induced by the two set of quadratic relations is known as *double shuffle relations* (see for example [Rac02]).

More recently, in [Fur08], Furusho proved that (III) implies the double shuffle relations. Seeing this fact directly on the coefficients is not easy because one has to find the "right linear combination". Although one can give the first example in weight 3 (see below), already in degree 4 one has to look at 211 relations ... Even looking only at the relations coming from multiplicative generators of $V(\mathcal{M}_{0,5})$ is difficult. However, Theorem 2.15 tells us that no information is lost between relation (III) and the family of relations given by (13). Thus, using Furusho's theorem, this family of relations implies the double shuffle relations.

Using a more suitable basis to write the relations, one that would give "nice" multiplicative generators for $V(\mathcal{M}_{0,5})$, or one coming from a "simple" basis of $V(\mathcal{M}_{0,5})$, may help to progress in the direction of the not known implication

"Double shuffle" implies (III).

However, this is not certain. A global approach (interpreting the series shuffle relations as a group-like property as in [Rac02] or in [Fur08]) or a geometric approach could be better.

Example 4.1. In weight 2, double shuffle relations do not give extra relations between multiple zeta values. They tell us the values of the second regularization of $\zeta^*(1,1)$: $\zeta^*(1,1) = \zeta(2)/2$, which is different from the *shuffle* regularization $\zeta^{ш}(1,1) = \zeta^{ш}(Y,Y) = 0$.

In weight 3, the double shuffle relations lead to $\zeta(3,1) = \zeta(2)$, which can be written as

$$\zeta^{ш}(X_0X_0X_1) = \zeta^{ш}(X_0X_1X_1).$$

This equality is a direct consequence of the duality relation; however, to recover it from Table 3, one needs to use 3 relations. Indeed, using the coefficients of monomials $X_{45}X_{24}X_{24}$, $X_{24}X_{45}X_{45}$, $X_{34}X_{45}X_{45}$, one finds

$$\zeta^{ш}(X_0X_1X_1) = \zeta^{ш}(X_1X_0X_0) = \zeta^{ш}(X_1X_1X_0) = \zeta^{ш}(X_0X_0X_1).$$

4.2. **Degree 1, 2 and 3.** Here one can find the explicit relations given by the pentagon equation ($\mathrm{III}_{\mathrm{KZ}}$) in low degree. Writing the product

$$\Phi_{KZ}(X_{12},X_{23})\Phi_{KZ}(X_{34},X_{45})\Phi_{KZ}(X_{51},X_{12})\Phi_{KZ}(X_{23},X_{34})$$
$$\Phi_{KZ}(X_{45},X_{51}) = \sum_{b_4} C_{b_4} b_4$$

in the basis B_4, the following tables give the relation $C_{b_4} = 0$ in terms of regularized multiple zeta values.

Let $B_4^{\deg=i}$ denote the family of elements in B_4 with degree equal to i. For any $S \subset B_4$, one defines S^* to be the set $\{b^* \mid b \in S\}$. Let N be an integer, $N \geqslant 1$. A sequence $\{S_1, \dots, S_N\}$ with $S_i \subset B_4^{\deg=i}$ is called *a set of multiplicative generators up to degree* N if for every $i = 1, \dots, N$ and every element ω of degree i in $V(\mathcal{M}_{0,5})$, ω is a linear combination of shuffles of elements in $\{1\} \cup S_1^* \cup \cdots S_i^*$. Let γ' be a path in the standard cell homotopically equivalent to $\gamma = p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$, and let f_1 and f_2 be two elements in $V(\mathcal{M}_{0,5})$. Then it is a property of iterated integrals ([Che73]) that

$$\left(\int_{\gamma'} f_1\right)\left(\int_{\gamma'} f_2\right) = \left(\int_{\gamma'} f_1 ш f_2\right).$$

Now, using Corollary 3.15, one deduces that

$$\left(\int_{\gamma} \mathrm{Reg}(f_1, \gamma)\right)\left(\int_{\gamma} \mathrm{Reg}(f_2, \gamma)\right) = \left(\int_{\gamma} \mathrm{Reg}(f_1 ш f_2, \gamma)\right).$$

In particular the family of relations

$$\forall b_4 \in B_4,\, b_4 \neq 1 \qquad \int_{\gamma} \mathrm{Reg}(b_4^*, \gamma) = 0$$

up to degree N is induced by

$$\forall i = 1, \dots N, \quad \forall s \in S_i, \qquad \int_{\gamma} \mathrm{Reg}(s^*, \gamma) = 0$$

for any set of multiplicative generators $\{S_1, \dots, S_N\}$ up to degree N. More precisely, let an element b_4 in B_4 be of degree less than or equal to N. The corresponding relation between multiple zeta values given at Equation (14) is exactly (Cf. Theorem 3.16)

$$\int_{\gamma} \mathrm{Reg}(b_4^*, \gamma) = 0.$$

Now, we write b_4^* in terms of multiplicative generators

$$b_4^* = \sum_{k=1}^{M} \lambda_k s_{i_k}^* ш s_{j_k}^*$$

with $s_{i_k}^*$, $s_{j_k}^*$ in $\{1\} \cup S_1^* \cup \cdots S_N^*$. Using the previous discussion, one has

$$\begin{aligned}\int_{\gamma} \mathrm{Reg}(b_4^*, \gamma) &= \sum_{k=1}^{M} \lambda_k \int_{\gamma} \mathrm{Reg}(s_{i_k}^* ш s_{j_k}^*, \gamma) \\ &= \sum_{k=1}^{M} \lambda_k \left(\int_{\gamma} \mathrm{Reg}(s_{i_k}^*, \gamma)\right)\left(\int_{\gamma} \mathrm{Reg}(s_{j_k}^*, \gamma)\right).\end{aligned}$$

Thus, the relation corresponding to b_4 is a consequence of the shuffle relations for the MZV and of the relations corresponding to the s_{i_k} and the s_{j_k}.

In degree 1 the basis is given by the letters X_{34}, X_{45}, X_{24}, X_{12} and X_{23}. The corresponding relations (equivalent to ($\mathrm{III}_{\mathrm{KZ}}$)) are given in Table 1.

In degree 2 the basis B_4 is given by 19 monomials, but we have only 4 multiplicative generators and the corresponding relations are given in Table 2. In degree 3 there are 10 multiplicative generators and the corresponding relations are given in Table 3.

The code used to produce the relations is given (and commented) in the next section.

Example 4.2. The monomial $b = X_{23}X_{12}$ is an element of the basis B_4 but is not part of the chosen weight 2 multiplicative generators of Table 2. Its dual element in $V(\mathcal{M}_{0,5})$ is given by

$$b^* = [\omega_{23}|\omega_{12}] = [\omega_{23}] ш [\omega_{12}] - [\omega_{12}|\omega_{23}].$$

As previously, let γ denote the path $p_{35} \circ p_{52} \circ p_{24} \circ p_{41} \circ p_{13}$. Computing the iterated integral $\int_\gamma \mathrm{Reg}([\omega_{23}|\omega_{12}], \gamma)$, one finds

$$0 = \int_\gamma \mathrm{Reg}([\omega_{23}|\omega_{12}], \gamma) = -\zeta^ш(X_1X_0) - \zeta^ш(X_0X_1) + \zeta^ш(X_1)^2. \tag{26}$$

In the other hand, the relations given by the iterated integrals of $[\omega_{23}]$, $[\omega_{12}]$ and $[\omega_{12}|\omega_{23}]$ are (see Tables 1 and 2)

$$0 = \int_\gamma \mathrm{Reg}([\omega_{23}], \gamma) = 2\left(\zeta^ш(X_0) - \zeta^ш(X_1)\right), \tag{27}$$

$$0 = \int_\gamma \mathrm{Reg}([\omega_{23}], \gamma) = \zeta^ш(X_0) - \zeta^ш(X_1) \tag{28}$$

and

$$\begin{aligned} 0 = \int_\gamma \mathrm{Reg}([\omega_{12}|\omega_{23}], \gamma) &= 2\zeta^ш(X_0)^2 - 2\zeta^ш(X_1)\zeta^ш(X_0) \\ &\quad + \zeta^ш(X_1)^2 - \zeta^ш(X_0X_1) - \zeta^ш(X_1X_0). \end{aligned} \tag{29}$$

Multiplying Equations (27) and (28) and subtracting Equation (29), one finds

$$0 = -2\zeta^ш(X_0)\zeta^ш(X_1) + \zeta^ш(X_1)^2 + \zeta^ш(X_0X_1) + \zeta^ш(X_1X_0).$$

Using the shuffle relation on the product $\zeta^ш(X_0)\zeta^ш(X_1)$, one gets

$$-\zeta^ш(X_1X_0) - \zeta^ш(X_0X_1) + \zeta^ш(X_1)^2 = 0,$$

which is exactly the relation given by the iterated integral $\int_\gamma \mathrm{Reg}([\omega_{23}|\omega_{12}], \gamma)$ at Equation (26). Here, we used the shuffle relation on the term

$$-2\zeta^ш(X_0)\zeta^ш(X_1)$$

because this term corresponds to the following integrals

$$\int_{p_{35}} \mathrm{Reg}([\omega_{23}] ш [\omega_{12}], p_{35}) = \left(\int_{p_{35}} \mathrm{Reg}([\omega_{23}], p_{35})\right)\left(\int_{p_{35}} \mathrm{Reg}([\omega_{12}], p_{35})\right)$$

and

$$\int_{p_{24}} \mathrm{Reg}([\omega_{23}] ш [\omega_{12}], p_{24}) = \left(\int_{p_{24}} \mathrm{Reg}([\omega_{23}], p_{24})\right)\left(\int_{p_{24}} \mathrm{Reg}([\omega_{12}], p_{24})\right).$$

Example 4.3. In weight 3, let us consider the monomial $b = X_{24}X_{23}X_{12}$, which is an element of the basis B_4, without being one of the chosen multiplicative generators of Table 3. Its dual element b^* is given by

$$b^* = [\omega_{24}|\omega_{23}|\omega_{12}] + [\omega_{23}|\omega_{24}|\omega_{12}] + [\omega_{23}|\omega_{12}|\omega_{24}] = [\omega_{24}] ш [\omega_{23}|\omega_{12}].$$

The element $[\omega_{23}|\omega_{12}]$ in $V(\mathcal{M}_{0,5})$ is dual to the monomial $X_{23}X_{12}$ which is not an element of the chosen weight 2 multiplicative generators (see Table 2). However, we explained in the previous example (Example 4.2) how to derive the relation corresponding to $X_{23}X_{12}$ from the relations corresponding to $X_{23}X_{12}$, X_{23} and X_{12}.

As previously, let γ denotes the path $p_{35}\circ p_{52}\circ p_{24}\circ p_{41}\circ p_{13}$. The complete relation given by the iterated integral $\int_\gamma \mathrm{Reg}(b^*,\gamma)$ is

$$\begin{aligned}(30)\quad &-\zeta^{ш}(X_1)^3+2\zeta^{ш}(X_1)\zeta^{ш}(X_0X_1)-\zeta^{ш}(X_0)\zeta^{ш}(X_1X_0)\\ &+2\zeta^{ш}(X_1)\zeta^{ш}(X_1X_0)-2\zeta^{ш}(X_0X_0X_1)-\zeta^{ш}(X_0X_1X_0)=0.\end{aligned}$$

The relations given by the iterated integral of $[\omega_{24}]$ and $[\omega_{23}|\omega_{12}]$ are respectively

$$\zeta^{ш}(X_0)-\zeta^{ш}(X_1)=0 \tag{31}$$

and

$$-\zeta^{ш}(X_1X_0)-\zeta^{ш}(X_0X_1)+\zeta^{ш}(X_1)^2=0. \tag{32}$$

Multiplying those two equations one finds

$$\begin{aligned}(33)\quad &-\zeta^{ш}(X_1X_0)\zeta^{ш}(X_0)-\zeta^{ш}(X_0X_1)\zeta^{ш}(X_0)+\zeta^{ш}(X_1)^2\zeta^{ш}(X_0)+\\ &\zeta^{ш}(X_1X_0)\zeta^{ш}(X_1)+\zeta^{ш}(X_0X_1)\zeta^{ш}(X_1)-\zeta^{ш}(X_1)^3=0.\end{aligned}$$

Now, using shuffle relations

$$-\zeta^{ш}(X_0X_1)\zeta^{ш}(X_0)=-2\zeta^{ш}(X_0X_0X_1)-\zeta^{ш}(X_0X_1X_0)$$

and

$$\zeta^{ш}(X_1)^2\zeta^{ш}(X_0)=\zeta^{ш}(X_1X_0)\zeta^{ш}(X_1)+\zeta^{ш}(X_0X_1)\zeta^{ш}(X_1),$$

one recovers the relation corresponding to $X_{24}X_{23}X_{12}$ given in Equation (30). As in the previous example, using the shuffle relations between multiple zeta values for some products corresponds to the shuffle relation between some products of iterated integrals.

One should also remark that it is possible to recover directly from Table 3 the relation

$$-2\zeta^{ш}(X_0X_0X_1)-\zeta^{ш}(X_0X_1X_0)=0$$

which is equivalent to Equation (30) as $\zeta^{ш}(X_0)=\zeta^{ш}(X_1)=0$. In order to do so, one uses the relations given by the monomials $X_{34}X_{34}X_{45}$ and $X_{24}X_{34}X_{45}$.

Monomials	Dual elements in $V(\mathcal{M}_{0,5})$	Relations
X_{12}	$[\omega_{12}]$	$\zeta^{ш}(X_0)-\zeta^{ш}(X_1)=0$
X_{23}	$[\omega_{23}]$	$2\left(\zeta^{ш}(X_0)-\zeta^{ш}(X_1)\right)=0$
X_{24}	$[\omega_{24}]$	$\zeta^{ш}(X_0)-\zeta^{ш}(X_1)=0$
X_{34}	$[\omega_{34}]$	$2\left(\zeta^{ш}(X_0)-\zeta^{ш}(X_1)\right)=0$
X_{45}	$[\omega_{45}]$	$\zeta^{ш}(X_0)-\zeta^{ш}(X_1)=0$

TABLE 1. Explicit set of relations equivalent to $(\mathrm{III}_{\mathrm{KZ}})$ in degree 1

Monomials $b_4 \in B_4$	Dual elements in $V(\mathcal{M}_{0,5})$ $b_4^* = \sum l_{b_4,W}\omega_W$	Relations
$X_{24}X_{45}$	$-[\omega_{12}\vert\omega_{24}] + [\omega_{24}\vert\omega_{45}]$	$\zeta^{ш}(X_0)\,\zeta^{ш}(X_1) - \zeta^{ш}(X_1)^2 = 0$
$X_{24}X_{34}$	$-[\omega_{12}\vert\omega_{24}] + [\omega_{23}\vert\omega_{24}] - [\omega_{23}\vert\omega_{34}] + [\omega_{24}\vert\omega_{34}]$	$-\zeta^{ш}(X_0)^2 + \zeta^{ш}(X_1)\,\zeta^{ш}(X_0) - 2\zeta^{ш}(X_1)^2 + \zeta^{ш}(X_0X_0) + \zeta^{ш}(X_0X_1) + \zeta^{ш}(X_1X_0) + \zeta^{ш}(X_1X_1) = 0$
$X_{34}X_{45}$	$[\omega_{34}\vert\omega_{45}]$	$2\zeta^{ш}(X_0)^2 - \zeta^{ш}(X_1)\,\zeta^{ш}(X_0) - \zeta^{ш}(X_0X_1) - \zeta^{ш}(X_1X_0) = 0$
$X_{12}X_{23}$	$[\omega_{12}\vert\omega_{23}]$	$2\zeta^{ш}(X_0)^2 - 2\zeta^{ш}(X_1)\,\zeta^{ш}(X_0) + \zeta^{ш}(X_1)^2 - \zeta^{ш}(X_0X_1) - \zeta^{ш}(X_1X_0) = 0$

Table 2. Explicit set of relations equivalent to ($\mathrm{III}_{\mathrm{KZ}}$) in degree 2

Monomials	Relations
$X_{34}X_{24}X_{24}$	$-\zeta^{ш}(X_0X_0X_1) - \zeta^{ш}(X_0X_1X_0) - \zeta^{ш}(X_1X_0X_0) = 0$
$X_{12}X_{23}X_{23}$	$\zeta^{ш}(X_0X_1X_1) - \zeta^{ш}(X_1X_0X_0) = 0$
$X_{34}X_{45}X_{45}$	$\zeta^{ш}(X_0X_1X_1) - \zeta^{ш}(X_1X_0X_0) = 0$
$X_{45}X_{24}X_{24}$	$\zeta^{ш}(X_0X_1X_1) - \zeta^{ш}(X_1X_0X_0) = 0$
$X_{12}X_{12}X_{23}$	$\zeta^{ш}(X_1X_1X_0) - \zeta^{ш}(X_0X_0X_1) = 0$
$X_{34}X_{34}X_{45}$	$\zeta^{ш}(X_1X_1X_0) - \zeta^{ш}(X_0X_0X_1) = 0$
$X_{24}X_{45}X_{45}$	$\zeta^{ш}(X_1X_1X_0) - \zeta^{ш}(X_1X_0X_0) = 0$
$X_{24}X_{34}X_{34}$	$\zeta^{ш}(X_0X_0X_1) + \zeta^{ш}(X_0X_1X_0) - \zeta^{ш}(X_0X_1X_1) + \zeta^{ш}(X_1X_0X_0) + \zeta^{ш}(X_1X_1X_0) = 0$
$X_{24}X_{45}X_{34}$	$\zeta^{ш}(X_1X_0X_0) + \zeta^{ш}(X_1X_0X_1) + \zeta^{ш}(X_1X_1X_0) = 0$
$X_{24}X_{34}X_{45}$	$\zeta^{ш}(X_0X_1X_0) + 2\zeta^{ш}(X_1X_1X_0) = 0$

Table 3. Explicit set of relations equivalent to ($\mathrm{III}_{\mathrm{KZ}}$) in degree 3 where we already have used the relations $\zeta^{ш}(X_0^k) = \zeta^{ш}(X_1^k) = 0$.

Monomials $b_4 \in B_4$	Dual elements in $V(\mathcal{M}_{0,5})$ $b_4^* = \sum l_{b_4,W}\omega_W$
$X_{34}X_{24}X_{24}$	$[\omega_{12}\vert\omega_{24}\vert\omega_{24}] + [\omega_{23}\vert\omega_{12}\vert\omega_{24}] - [\omega_{23}\vert\omega_{23}\vert\omega_{24}] + [\omega_{23}\vert\omega_{23}\vert\omega_{34}] - [\omega_{23}\vert\omega_{24}\vert\omega_{24}] + [\omega_{23}\vert\omega_{34}\vert\omega_{24}] + [\omega_{34}\vert\omega_{24}\vert\omega_{24}]$
$X_{12}X_{23}X_{23}$	$[\omega_{12}\vert\omega_{23}\vert\omega_{23}]$
$X_{34}X_{45}X_{45}$	$[\omega_{34}\vert\omega_{45}\vert\omega_{45}]$
$X_{45}X_{24}X_{24}$	$[\omega_{12}\vert\omega_{24}\vert\omega_{24}] + [\omega_{45}\vert\omega_{24}\vert\omega_{24}]$
$X_{12}X_{12}X_{23}$	$[\omega_{12}\vert\omega_{12}\vert\omega_{23}]$
$X_{34}X_{34}X_{45}$	$[\omega_{34}\vert\omega_{34}\vert\omega_{45}]$
$X_{24}X_{45}X_{45}$	$[\omega_{12}\vert\omega_{12}\vert\omega_{24}] - [\omega_{12}\vert\omega_{24}\vert\omega_{45}] + [\omega_{24}\vert\omega_{45}\vert\omega_{45}]$
$X_{24}X_{34}X_{34}$	$[\omega_{12}\vert\omega_{12}\vert\omega_{24}] - [\omega_{12}\vert\omega_{23}\vert\omega_{24}] + [\omega_{12}\vert\omega_{23}\vert\omega_{34}] - [\omega_{12}\vert\omega_{24}\vert\omega_{34}] - [\omega_{23}\vert\omega_{12}\vert\omega_{24}] + [\omega_{23}\vert\omega_{23}\vert\omega_{24}] - [\omega_{23}\vert\omega_{23}\vert\omega_{34}] + [\omega_{23}\vert\omega_{24}\vert\omega_{34}] - [\omega_{23}\vert\omega_{34}\vert\omega_{34}] + [\omega_{24}\vert\omega_{34}\vert\omega_{34}]$
$X_{24}X_{45}X_{34}$	$[\omega_{12}\vert\omega_{12}\vert\omega_{24}] - [\omega_{12}\vert\omega_{23}\vert\omega_{24}] + [\omega_{12}\vert\omega_{23}\vert\omega_{34}] - [\omega_{12}\vert\omega_{24}\vert\omega_{34}] + [\omega_{24}\vert\omega_{45}\vert\omega_{34}]$
$X_{24}X_{34}X_{45}$	$[\omega_{12}\vert\omega_{12}\vert\omega_{24}] - [\omega_{12}\vert\omega_{24}\vert\omega_{45}] - [\omega_{23}\vert\omega_{12}\vert\omega_{24}] + [\omega_{23}\vert\omega_{24}\vert\omega_{45}] - [\omega_{23}\vert\omega_{34}\vert\omega_{45}] + [\omega_{24}\vert\omega_{34}\vert\omega_{45}]$

TABLE 4. Correspondence between ten multiplicative generators of weight 3 in $U\mathfrak{B}_5$ and their dual elements in $V(\mathcal{M}_{0,5})$

5. Appendix : algorithm

5.1. **Comments.** The above computations were done using the software Mathematica because its replacement rules and pattern recognition are very efficient dealing with words. In this section, the algorithms used to produce the tables from the previous sections are commented.

The naive algorithms described below were originally intended to provide help in guessing the family of relations (14) given by the pentagon relation. Concentrating our attention on understanding (14), proving it and explaining the connection with the bar construction on $\mathcal{M}_{0,5}$, the author did not make a particular effort to improve the algorithms (and their results).

5.2. **Law, relations, and basis.** Using Mathematica, we need to define a new *NonCommutativeMultiply* function which behaves like the desired multiplicative law for a polynomial algebra with non-commutative variables. This is done using Mathematica's elementary operations such as pattern recognition and replacement rules. All the non-commutative products used in the algorithms below are understood as this new *NonCommutativeMultiply* function.

In order to write words in $\{X_{12}, X_{23}, X_{34}, X_{45}, X_{51}\}^*$ in the basis B_4, we need to use the relations in $U\mathfrak{B}_5$ and thus to implement the functions $REl51$ and $Relcom$.

- The function $Rel51$ writes the letter X_{51} in terms of X_{23}, X_{24}, X_{34}:

$$Rel51: \quad X_{51} \longmapsto X_{23} + X_{24} + X_{34}$$

- The function $Relcom$ uses the commutation relations to write a product $X_{ij}X_{kl}$ with X_{12} or X_{23} on the right side. It does nothing to the product $X_{ij}X_{kl}$ if it is a word in the letters X_{12}, X_{23} or if it is a word in the letters X_{34}, X_{45} and X_{24}. Beginning with a word in $\mathcal{W}$ and iterating applications of the function $Relcom$, one obtains its decomposition in the basis B_4.

$$\begin{aligned}
Relcom: \quad & X_{12}X_{kl} \longmapsto X_{kl}X_{12} \quad \text{for } k=3 \text{ and } l=4, \text{ or } k=4, \text{ and } l=5\\
& X_{23}X_{45} \longmapsto X_{45}X_{23}\\
& X_{12}X_{24} \longmapsto (X_{24}+X_{34}+X_{45})X_{24} - X_{24}(X_{24}+X_{34}+X_{45})\\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + X_{24}X_{12}\\
& X_{23}X_{24} \longmapsto X_{24}X_{34} - X_{34}X_{24} + X_{24}X_{23}\\
& X_{23}X_{34} \longmapsto X_{34}X_{24} - X_{24}X_{34} + X_{34}X_{23}
\end{aligned}$$

Computing up to a fixed weight n, we consider a basis restricted to weight n and less, and we define functions $BX0X1$ and B_4 which give respectively the list of the corresponding monomials.

- $BX0X1(n) :=$ List of words $W \in \mathcal{W}_{0,1}$ with $|W| \leqslant n$.
- $B_4(n) :=$ List of words $W = W_1W_2$ with $W_1 \in {}_{24}\mathcal{W}_{34,45}$, $W_2 \in \mathcal{W}^{12,23}$ and $|W| \leqslant n$.

Then, for any given A in $U\mathfrak{B}_5$ given as

$$A = \sum_{\substack{W\in\{X_{51},X_{34},X_{45},X_{12},X_{23}\}^*,\\ |W|\leqslant n}} a_W W$$

one can write A in the basis B_4 by using the function $DecB_4$ below:

- $DecB_4 :=$
  - $A_1 := Rel51(A)$ and expand A_1 as $\sum_{W\in\mathcal{W}\,|W|\leqslant n} b_W W$.
  - Do $A_1 := Relcom(A_1)$ until $A_1 = \sum_{W\in B_4\,|W|\leqslant n} c_W W$.

This function is defined using the build-in function *Expand* and *Collect* together with the previously defined functions. For later use, we need a function $Deg(A,n)$ that truncates A at weight n.

5.3. **Exponential, associator.** Working up to a fixed weight n, we now construct a function that takes two variables A and B and an integer n as inputs and gives as output a general polynomial $\Phi_n(A,B)$ of degree n with formal coefficients

$$\Phi_n(A,B) = 1 + \sum_{\substack{W \in \mathcal{W}_{0,1},\, \{A,B\}^* \neq \emptyset \\ |W| \leqslant n}} (-1)^{dp(W)} Z_{\bar{W}} W,$$

where $\bar{W}$ is obtained from W by sending A to X_0 and B to X_1.

We also define a non-commutative exponential up to degree n

$$Exp_n(A) = \sum_{0 \leqslant k \leqslant n} \frac{A^k}{k!}.$$

5.4. **Development of the associator relations.** We detail here how we develop the hexagonal and pentagonal relations.

In order to develop the hexagonal relation

$$e^{p*X_0}\Phi_n(X_\infty, X_0)e^{p*X_\infty}\Phi_n(X_1, X_\infty)e^{p*X_1}\Phi_n(X_0, X_1)$$

truncated in degree n and expand in the basis given by the words in X_0 and X_1. We proceed as follows:

(1) We compute the successive products keeping only the terms of weight less or equal to n. That is, we compute

$$\begin{aligned} P_1 &= Deg(e^{pX_0}\Phi_n(X_\infty, X_0), n), \\ P_2 &= Deg(P_1 e^{pX_\infty}, n), \\ &\dots \\ P_6 &= Deg(P_5\Phi_n(X_0, X_1), n) \end{aligned}$$

(2) Then, we apply $X_\infty \longmapsto -X_0 - X_1$ and $p \longmapsto i\pi$ to P_6.

(3) Finally, we expand the expression and collect the terms of the sum with respect to the list $BX0X1(n)$ and obtain an expression

$$\sum_{W \in \mathcal{W}_{0,1},\, |W| \leqslant n} a_W W.$$

The coefficients a_W are expressed as a sum of products of a rational coefficient, a power of $i\pi$ and a product of Z_U for U in $\mathcal{W}_{0,1}$. Formally replacing Z_U by $\zeta^{\mathrm{m}}(U)$, the set of relations (9) is given by

$$a_W = 0 \qquad (W \neq \emptyset).$$

Similarly, in order to find the set of relations (14) arising from the 5-cycle equation ($\mathrm{III_{KZ}}$), we expand the product

$$Penta = \Phi_n(X_{12}, X_{23})\Phi_n(X_{34}, X_{45})\Phi_n(X_{51}, X_{12})\Phi_n(X_{23}, X_{34})\Phi_n(X_{45}, X_{51}),$$

computing the successive products and keeping only the part of weight less or equal to n at each step.

Then, we develop the corresponding expression with the variables X_{12}, X_{23}, X_{34}, X_{45}, X_{51} in the basis B_4, applying the function $DecB_4$ to the expression $Penta$, to obtain an expression of the form

$$\sum_{b \in B_4,\, |b| \leqslant n} a'_b b.$$

The coefficients a'_b are a sum of products of Z_U for U in $\mathcal{W}_{0,1}$. One can formally replace Z_U by $\zeta^{ш}(U)$ and obtain the set of relations (14) setting $a'_b = 0$ for b not equal to 1.

5.5. **Using for** $(\mathrm{III}_{\mathrm{KZ}})$ **the equivalent set of relations given in** (14)**.** We describe here how to obtain the family of relations (14) up to degree n, that is:

For any $b \in B_4$ with $|b| \leqslant n$, $b \neq 1$

$$\sum_{W \in \mathcal{W}} l_{b,W} C_{5,W} = 0,$$

by first generating the coefficients $C_{5,W}$ and then the coefficient $l_{b,W}$.

In order to compute the coefficients $C_{5,W}$ for any word W in $\mathcal{W}$, we first construct a function $Decw$ that takes a word as input and gives as output all the possibilities to cut it into five sub-words.

$$Decw(W) := \text{List of decomposition } (U_1, \ldots, U_5) \text{ such that } U_1 \cdots U_5 = W.$$

The function $Decw$ is built inductively by first giving the list of all decompositions $U_1 U_2 = W$, then iterating the process on each U_1 and so forth.

Then, we implement functions corresponding to the ρ_i (Definition 2.13) by programming the behavior on the letters as follow

$$\begin{aligned}
rho(i, X_{12}) :=& X_0 \text{ if } i = 1,\ X_1 \text{ if } i = 3 \text{ and } 0 \text{ otherwise},\\
rho(i, X_{23}) :=& X_0 \text{ if } i = 2, 3,\ X_1 \text{ if } i = 1, 5 \text{ and } 0 \text{ otherwise},\\
rho(i, X_{45}) :=& X_0 \text{ if } i = 5,\ X_1 \text{ if } i = 2 \text{ and } 0 \text{ otherwise},\\
rho(i, X_{34}) :=& X_0 \text{ if } i = 2, 3\, X_1 \text{ if } i = 4, 5 \text{ and } 0 \text{ otherwise},\\
rho(i, X_{24}) :=& X_0 \text{ if } i = 3,\ X_1 \text{ if } i = 5 \text{ and } 0 \text{ otherwise},
\end{aligned}$$

which extends to words. The function $Zrho$ takes as input i and a word U_i in $\mathcal{W}$ and gives the coefficient

$$(-1)^{dp(\rho_i(U_i))} \zeta^{ш}(\rho_i(U_i)).$$

- $Zrho(i, U_i) :=$
  - Do $V = rho(i, U_i)$ and $s = dp(V)$
  - output : $(-1)^s \zeta^{ш}(V)$

Now, from a decomposition

$$U_1 \cdots U_5 = W$$

we can recover the coefficient

$$(-1)^{dp_1(U_1)+dp_2(U_2)+dp_3(U_3)+dp_4(U_4)+dp_5(U_5)} \\ \zeta^{ш}(\rho_1(U_1))\zeta^{ш}(\rho_2(U_2))\zeta^{ш}(\rho_3(U_3)\zeta^{ш}(\rho_4(U_4))\zeta^{ш}(\rho_5(U_5)),$$

that is

$$Z(U_1, U_2, U_3, U_4, U_5) := \prod_{i=1}^{5} Zrho(i, U_i).$$

Using functions $Decw$ and Z, we now compute the sum over the whole set of decompositions and obtain a function that gives the coefficient $C_{5,W}$:

$$C5(W) := \sum_{(U_1, \ldots, U_5) \in Decw(W)} Z(U_1, U_2, U_3, U_4, U_5).$$

We now compute the $l_{b,W}$ coefficients up to some weight by the following algorithm:

- Begin with $L :=$ List of words $W \in \mathcal{W}$, $|W| \leqslant n$.
- $L1 :=$ for each element in L apply $DecB_4$
- $L2 :=$ for each element in $L1$ replace $\sum_{b \in B_4} l_{b,W} b$ by the list of the corresponding $l_{b,W}$.
- output : $L2$.

One can then compute for any $b \in B_4$ with $|b| \leqslant n$, $b \neq 1$

$$\sum_{W \in \mathcal{W}} l_{b,W} C_{5,W}$$

which is the L.H.S. of (14).

Remark 5.1. One could imitate the algorithm that gives $C_{5,W}$ in order to recover the pentagon relation using the bar construction side of the story. The decomposition function $Decw$ could be directly reused to cut a bar symbol ω_W in five pieces. The rho function corresponds to the implementation of the regularization Reg on the u_{ij}. In order to recover the pentagon relation from

$$\forall b^* \in B^* \qquad \int_\gamma \mathrm{Reg}(b^*, \gamma) = 0,$$

B^* being a basis of $V(\mathcal{M}_{0,5})$, one will have to implement linearity and the correspondence between formal bar symbols and their iterated integrals. The latter should be similar to the function $Zrho$ but one may need to be careful with possible signs.

5.6. **Remarks.** The author, having recently discovered the software Sagemath, thinks that it may be easier to do the computations with Sagemath. This is because Sagemath seems to work well with non-commutative formal power series and it has large libraries to deal with words.

In [BO96], M. Bigotte and N.E. Oussous have described a Maple package to work with non-commutative power series. However, it was not yet possible to have access to this package when this work began.

References

[BGL10] Francis Brown, Herbert Gangl, and Andrey Levin, *Polygonal algebraic cylce and moduli space of curve*, Informal communication, 2010.

[BO96] M. Bigotte and N.E. Oussous, *Algbre non commutative et algbre de lie libre en maple*, RCWA 96, Proceedings PR 801=96, Institut de Recherche Franco-Allemand de Saint Louis, 1996, pp. 24.1–24.24.

[Bro09] Francis C. S. Brown, *Multiple zeta values and periods of moduli spaces* $\overline{\mathfrak{M}}_{0,n}$, Ann. Sci. Éc. Norm. Supér. (4) **42** (2009), no. 3, 371–489.

[Che73] Kuo-tsai Chen, *Iterated integrals of differential forms and loop space homology*, Ann. of Math. (2) **97** (1973), 217–246.

[Dri91] V. G. Drinfel'd, *On quasitriangular quasi-Hopf algebras and on a group that is closely connected with* $\mathrm{G}al(\overline{\mathbb{Q}}/\mathbb{Q})$, translation in Leningrad Math. J. **2** (1991), no. 4, 829–860.

[Fur03] Hidekazu Furusho, *The multiple zeta value algebra and the stable derivation algebra*, Publ. Res. Inst. Math. Sci. **39** (2003), no. 4, 695–720.

[Fur08] Hidekazu Furusho, *Double shuffle relation for associators*, http://arxiv.org/abs/0808.0319, 2008.

[Fur10] Hidekazu Furusho, *Pentagon and hexagon equations*, Ann. of Math. (2) **171** (2010), no. 1, 545–556.

[GL98] Jorge Gonzales-Lorca, *Série de drinfeld, monodromie et algèbres de hecke,*, Ph.D. thesis, École Normale Spupérieure, Université Paris XI-Orsay, 1998.

[Iha90] Yasutaka Ihara, *Automorphisms of pure sphere braid groups and Galois representations*, The Grothendieck Festschrift, Vol. II, Progr. Math., vol. 87, Birkhäuser Boston, Boston, MA, 1990, pp. 353–373.

[IKZ06] Kentaro Ihara, Masanobu Kaneko, and Don Zagier, *Derivation and double shuffle relations for multiple zeta values*, Compos. Math. **142** (2006), no. 2, 307–338.

[LM96] Thang Tu Quoc Le and Jun Murakami, *Kontsevich's integral for the Kauffman polynomial*, Nagoya Math. J. **142** (1996), 39–65.

[Ohn99] Yasuo Ohno, *A generalization of the duality and sum formulas on the multiple zeta values*, J. Number Theory **74** (1999), no. 1, 39–43.

[Rac02] Georges Racinet, *Doubles mélanges des polylogarithmes multiples aux racines de l'unité*, Publ. Math. Inst. Hautes Études Sci. (2002), no. 95, 185–231.

[Zag94] Don Zagier, *Values of zeta functions and their applications*, First European Congress of Mathematics, Vol. II (Paris, 1992), Progr. Math., vol. 120, Birkhäuser, Basel, 1994, pp. 497–512.

Fachbereich Mathematik, Universität Duisburg-Essen, Campus Essen, Universitätsstrasse 2, 45117 Essen, Germany, ismael.souderes@uni-due.de